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Continuum Limit of a One-Dimensional Atomistic Energy Based on Local Minimization

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For atomistic energies, global minimization gives the wrong qualitative behaviour and therefore continuum limits should be formulated in terms of local minimization. In this paper, a possible process is suggested, to describe local minimization for a simple one-dimensional problem with body and surface energy. It is shown that an atomistic gradient flow evolution converges to a continuum gradient flow as the spacing between the atoms tends to zero. In addition, the convergence of local minimizers is investigated, in the case of both elastic deformation and fracture.

Key words and phrases: continuum limit, atomistic models, local minimization, gradient flows

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1 Introduction

Continuum limits of atomistic models have been considered by many authors, including Braides et al. using techniques of Γ-convergence [BDMG99, BG02] and E and Ming [EM04] considering only small deformations, but showing that Γ-convergence which is based on global energy minimization may not be the correct approach. The Γ-convergence approach is also rejected by Blanc et al. [BLBL02], who consider what is essentially pointwise convergence. Except for the fact that they consider far more general atomistic interactions and do not restrict themselves to one-dimensional systems, the continuum limit they is the same as the one we obtain in the present work. In fact, this paper may be seen as a small step towards a rigorous justification of the approach taken in [BLBL02].

The difficulty, which we try to address in this paper is that an atomistic model is typically a finite-dimensional system, so that, due to norm-equivalence, the term *local minimization* is perfectly well-defined. In the continuum limit, however, the choice of topology is crucial. For example, E and Ming[EM04] claim that under small external loads, there exists a $\mathrm{W}^{1,\infty}$-local minimizer, which is the limit of the correct atomistic minimizers.

Additionally, the non-convexity of the interaction potentials creates a large number of local minimizers. Already the simple one-dimensional energy (3.1) has a number of local minimizers which is at least proportional to the number of atoms, if the body force vanishes and the surface force is positive. We therefore require a selection criterion to choose the 'correct' local minimizer. This selection criterion should be the dynamics of the material.

In this paper, we choose simple gradient flow dynamics to study the problem. While a gradient flow may not be the physically correct evolution under which an equilibrium should be stable, it is, nevertheless, a significant improvement over the unphysical concept of global minimisation. Gradient flows are extensively used in computations; for example, in the quasi-continuum method it is used to identify local minimizers in quasistatic evolutions. Rieger and Zimmer [RZ] use a gradient flow in a space of Young measures as an approximation to a quasistatic evolution to model damage.

The structure of this paper is as follows. In Section 2 we review the approximation theory for gradient flows developed in [Ort05]. In Section 3, we define a simple atomistic energy E_h and establish the convergence of the H^1-gradient flow of E_h to the H^1-gradient flow of an appropriate continuum energy. The reason for this choice is a mathematical one: the strong topology is required to balance the non-convexity of the atomistic interaction potential. Finally, in Section 4, we investigate the convergence of the atomistic gradient flow evolutions to local minimizers of the atomistic energy as time tends to infinity, and the convergence of the resulting atomistic equilibria to an equilibrium of the continuum energy, which turns out to not be a local minimum. The examples we give raise some interesting questions concerning the concept of stable equilibria in the continuum setting.

We show in particular, that the equilibrium obtained in the elastic case is stable under $W^{1,\infty}$-perturbations, but it is not an H^1-local minimizer. We were, however, unable to construct a 'smooth' curve, starting in the equilibrium, along which the continuum energy decreases. If we were able to prove that no such curve exists, then the equilibrium would be stable under general 'smooth evolutions' thus showing that the choice of evolution is not so crucial after all, as long as the deformation remains close to an equilibrium.

2 Approximation of Gradient Flows

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 $\phi : \mathscr{H} \to (-\infty, \infty]$. If ϕ is Fréchet differentiable at a point u, we denote the representation of its derivative, i.e. its gradient, by $\phi'(u)$. Higher order derivatives are denoted for example by $\phi''(u; v_1, v_2)$, and so on. We denote the domain of definition of ϕ by $D(\phi) = \{u \in \mathscr{H} : \phi(u) < \infty\}$.

A curve $u \in C^1(a, b; \mathscr{H})$ is called a gradient flow of ϕ, if

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

In this paper, we are specifically interested in gradient flows of non-convex functionals. A recently identified 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 [AGS05]. We say that ϕ is λ-convex in $\mathscr{A}$, if there exists $\lambda \in \mathbf{R}$ such that

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

To obtain a better feel for the meaning of λ-convexity, consider the following simple Proposition, which is proven in [Ort05].

Proposition 1 *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 $\mathscr{A}$.*

In particular, if ϕ is differentiable at every point of $\mathscr{A}$ and satisfies

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

then ϕ is λ-convex in $\mathscr{A}$. If ϕ is twice differentiable at every non-extremal point of $\mathscr{A}$ and

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

then ϕ is λ-convex in $\mathscr{A}$.

If $\phi = \phi_1 + \phi_2$, where $\phi_i : \mathscr{A} \to (-\infty, +\infty]$, ϕ_1 is convex and ϕ_2 is λ-convex, then ϕ is λ-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

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

This inequality is the basis for a strong theory of gradient flows in metric spaces (then called curves of maximal slope) in Chapter 4 of [AGS05]. Note, for example, that it makes sense to consider $u, v \in \mathscr{A}$ only, instead of all of $\mathscr{H}$. Theorem 2 is a collection of results in [AGS05] translated to the Hilbert space setting.

Theorem 2 (Existence and uniqueness) *Let $\mathscr{A}$ be a convex subset of a Hilbert space $\mathscr{H}$ and let $\phi : \mathscr{A} \to (-\infty,\infty]$ be (strongly) lower semi-continuous and λ-convex. For each $u_0 \in D(\phi)$, there exists a locally Lipschitz-continuous curve $u : [0,\infty) \to \mathscr{A}$ which is the unique solution of*

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

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

Based on the evolutionary variational inequality stated above, an abstract convergence theory for gradient flows in a general metric setting for possibly non-convex and non-differentiable functionals was developed in [Ort05]. Theorem 3 below is one result therein which is relevant for the Hilbert space setting in the present work.

Let $(\phi_h)_{h\in\mathbf{N}}$ be a family of functionals $\phi_h : \mathscr{A} \to (-\infty,\infty]$, which are *approximations* to the functional ϕ. To approximate gradient flows for ϕ, we compute gradient flows for ϕ_h and compare them, using (2.5) and Gronwall's Lemma. The result obtained by this procedure is the following.

Theorem 3 *Let $\mathscr{A}$ be a convex subset of a Hilbert space $\mathscr{H}$ and, for $h \in \mathbf{N}$, let $\phi, \phi_h : \mathscr{A} \to (-\infty,\infty]$ be functionals defined on $\mathscr{A}$. Let $u^0 \in D(\phi)$ and $u_h^0 \in D(\phi_h)$ be given initial values, and assume that following conditions are satisfied:*

(i) Lower Semi-continuity: *The functionals ϕ and ϕ_h ($h \in \mathbf{N}$) are lower semi-continuous.*

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

(iii) Equi-Coercivity: *There exists a point $u^* \in \mathscr{A}$ and $\epsilon > 0$ such that $\inf_{h\in\mathbf{N}} \inf_{v\in\mathscr{A},\|v-u^*\|\leq\epsilon} \phi_h(v) > -\infty$.*

(iv) Convergence of the initial data: $\sup_{h\in\mathbf{N}} \phi_h(u_h^0) < \infty$ *and* $\|u_h^0 - u^0\| \to 0$ *as* $h \to \infty$.

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

$$\limsup_{h\to\infty} \big(\phi(w_h) - \phi_h(w_h)\big) \leq 0, \text{ and } \phi(w_h) \leq c_1(1 + [\phi_h(w_h)]^+ + \|w_h\|^2).$$

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

$$\phi_h(v_h(t)) \to \phi(u(t)) \text{ and } \phi_h(v_h(t)) \leq c_2(1 + [\phi(u(t))]^+ + \|u(t)\|^2),$$

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

Then the gradient flows (in the sense of Definition 1) u_h of ϕ_h with initial values u_h^0 converge in $\mathrm{L}^\infty_{\mathrm{loc}}([0,\infty);\mathscr{H})$ to the gradient flow u of ϕ with initial value u^0.

We conclude this Section, by stating a result from [AGS05], concerning the implicit Euler approximation of a gradient flow.

Lemma 4 *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*

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

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.,

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

Then, $\bar{u}_\tau(t) \to u(t)$ for every $t \geq 0$, as $\tau \to 0$.

3 Convergence of an Atomistic Evolution

3.1 A simple atomistic energy

For each $h \in \mathbf{N}$ consider a chain of $h+1$ atoms, at positions $(u_i^h)_{i=0,\dots,h} \subset \mathbf{R}$, $u_0 = 0$. For each such configuration of the atomistic body, we define the potential energy

$$E_h((u_i^h)) = \sum_{j=1}^{h} \epsilon_h \left[J\left(\frac{u_j^h - u_{j-1}^h}{\epsilon_h}\right) - f_j^h(u_j^h + u_{j-1}^h)/2 \right] - g u_h^h, \tag{3.1}$$

where $\epsilon_h = 1/h$. $J = J(z)$ is a Lennard-Jones-type potential, satisfying

$$\begin{aligned} &J(z) \;=\; +\infty \text{ if } z \le 0 \text{ and } J(z) \to \infty \text{ as } z \to 0,\\ &J \text{ is strictly convex in } (0, z_1), \text{ and}\\ &\text{concave, increasing and bounded above in } (z_1, \infty),\\ &J'(1) = 0, \text{ and } J \in \mathrm{C}^2(0, +\infty), \end{aligned} \tag{3.2}$$

with $1 < z_1 < +\infty$. The family $(f_i^h)_{i=1,\dots,h}$ defines a linear body force, which is obtained by averaging an L^1 function, i.e.,

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

where $x_i^h = i/h$, for each $i \in \mathbf{Z}$. 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 $u_i^h \le M$, where $M \in (1, \infty]$.

Our goal, which we shall turn to in Section 4, is to find the stable equilibrium that the material would 'naturally' assume if we started in the reference configuration $u_i^h = x_i^h$ and then suddenly applied the forces (f_i^h), g. To achieve this we should consider the dynamics of the body and let time tend to infinity. Here, we postulate the dynamics to be an H^1-gradient flow of the functional. The choice of gradient flow was governed by the wish to analyze local minimization. The choice of topology – the strong H^1-topology – was necessary to make the continuum problem well-posed. The H^1-norm is required to balance out the non-convexity of the leading term in E_h. Note also, that even if we had a theory of gradient flows of non-convex functionals in weaker topologies at our disposal, Proposition 16 would suggest that on the continuum level such an evolution would give the wrong qualitative behaviour even for small applied loads.

We shall test the gradient flow model on the following question: How small does f, g have to be to retain elastic behaviour? In other words, how large do f, g have to be in magnitude so that damage or fracture occurs? In the atomistic setting, the point at which damage occurs is when $(u_i - u_{i-1})/\epsilon_h$ enters the concave region of the potential, compare also [BDMG99]. Fracture occurs when the atoms debond, i.e., $(u_i - u_{i-1})/\epsilon_h \gg z_1$. We are particularly interested in the continuum manifestation of these effects.

3.2 The H^1-gradient flow

Let us define

$$\begin{aligned} u_h'(x) &= \frac{u_i^h - u_{i-1}^h}{\epsilon_h} \quad \text{if } x \in (x_{i-1}^h, x_i^h), \text{ and} \\ u_h(x) &= \int_0^x u_h'(x)\,\mathrm{d}x. \end{aligned}$$

Then, u_h is the piecewise-affine interpolant of (u_i^h) and u_h' is its weak derivative, and we have in particular that $u_h \in \mathscr{A}_h$, the set of admissable atomistic deformations, which is defined as

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

Thus, we can rewrite E_h as

$$E_h(u_h) = \int_0^1 \big[J(u_h') - f_h u_h \big]\,\mathrm{d}x - g u_h(1) \qquad \text{for } u_h \in \mathscr{A}_h, \tag{3.3}$$

where f_h is the piecewise constant interpolant of f with

$$f_h(x) = f_h^i \ \text{ for } x \in (x_{i-1}, x_i). \tag{3.4}$$

We shall show below that E_h is λ-convex in the H^1-metric. Therefore, from Theorem 3, we expect the correct limit energy (in the gradient flow) to be

$$E(u) = \int_0^1 \big[J(u') - f u \big]\,\mathrm{d}x - g u(1),$$

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

In the subset $\mathscr{A}$, the H^1-seminorm is equivalent to the H^1-norm, and hence we may consider the gradient flow in the H^1-seminorm

$$|u|_{\mathrm{H}^1} = \|u'\|_{\mathrm{L}^2}.$$

In general, we will define either $\|\cdot\|_{\mathscr{A}} = \|\cdot\|_{\mathrm{H}^1}$ or $\|\cdot\|_{\mathscr{A}} = |\cdot|_{\mathrm{H}^1}$. Most of the results hold true for either choice, but there are some interesting differences. The following theorem states that the (atomistic) $\mathscr{A}$-norm gradient flow of E_h in $\mathscr{A}_h$ converges to the (continuum) $\mathscr{A}$-norm gradient flow of E in $\mathscr{A}$. We embed $\mathscr{A}_h$ in $\mathscr{A}$ by setting $E_h(u) = +\infty$ if $u \in \mathscr{A} \setminus \mathscr{A}_h$.

Theorem 5 *Let $u^0 \in D(E)$, and let $u_h^0 \in \mathscr{A}_h$ be the piecewise affine interpolant of u^0 with respect to the mesh (x_i^h). Then, the $\mathscr{A}$-gradient flow u_h of E_h with initial data u_h^0 converges in $\mathrm{L}^\infty_{\mathrm{loc}}([0,\infty);\mathscr{A})$ to the $\mathscr{A}$-gradient flow u of E with initial data u^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 3.

Lemma 6 *With respect to the $\mathscr{A}$-norm, the functionals E and E_h ($h \in \mathbf{N}$) are λ-convex in $\mathscr{A}$, with $\lambda = \min_{z>0} J''(z)$, and lower semi-continuous.*

Proof For the λ-convexity as well as the lower semi-continuity, 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 1, we define $F(z) = J(z) - (\lambda/2)z^2$. By the definition of λ, $F''(y) \geq 0$ whenever $y > 0$, hence F is convex in $(0,\infty)$. Since $F(z) = +\infty$ for $z \leq 0$, F is convex on $\mathbf{R}$.

Applying this result to E, let $v_t = (1-t)v_0 + tv_1$ for $v_0, v_1 \in \mathrm{H}^1(0,1)$, and consider

$$\begin{aligned} E(v_t) - \frac{\lambda}{2}\|v_t'\|_{\mathrm{L}^2}^2 &= \int_0^1 F(v_t')\,\mathrm{d}x \\ &\leq \int_0^1 (1-t)F(v_0) + tF(v_1)\,\mathrm{d}x \\ &= (1-t)\big(E(v_0) - \lambda/2\|v_0'\|_{\mathrm{L}^2}^2\big) + t\big(E(v_1) - \lambda/2\|v_1'\|_{\mathrm{L}^2}^2\big). \end{aligned}$$

Using Theorem 1, we obtain the E is λ-convex in $\mathscr{A}$. As E_h is the restriction of E to a convex set, we have the same result for E_h.

To prove the lower semi-continuity, consider the functional

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

where F is convex and lower semi-continuous. By a standard result (see for example Theorem 1 in [Dac89]), G is therefore sequentially lower semi-continuous, even in the weak topology of H^1. Since

$$E(u) = G(u) + \frac{\lambda}{2}\|u'\|_{\mathrm{L}^2} - \int_0^1 fu\,\mathrm{d}x - gu(1),$$

where the added terms are continuous in H^1, the result follows for the functional E. To see that E_h is lower semi-continuous, simply note that under the assumption that $f, g \equiv 0$, $E_h = E|_{\mathscr{A}_h}$ where $\mathscr{A}_h$ is convex and closed and hence the proof carries over to E_h as well. ■

Lemma 7 *If $f \in \mathrm{L}^1(0,1)$, then, for every $v \in \mathscr{A}$, we have that*

$$\Big| \int_0^1 (f_h - f) v \,\mathrm{d}x \Big| \le \|v\|_{\mathscr{A}} \|f - f_h\|_{\mathrm{L}^1(0,1)}, \text{ and}$$
$$\|f - f_h\|_{\mathrm{L}^1} \to 0 \quad \text{as } h \to 0,$$

where f_h is defined as in (3.4).

Proof Hölder's inequality gives

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

Using $v(0) = 0$, we also have

$$\|v\|_{\mathrm{L}^\infty} \le \|v'\|_{\mathrm{L}^1} \le \|v'\|_{\mathrm{L}^2} \le \|v\|_{\mathscr{A}},$$

which gives the first result. The convergence $\|f_h - f\|_{\mathrm{L}^1} \to 0$ follows from the fact that f_h is the L^2-projection of f onto the piecewise constant functions with respect to the mesh (x_i^h). For, let $f_\epsilon \in \mathrm{L}^2$ such that $\|f - f_\epsilon\|_{\mathrm{L}^1} \le \epsilon$, and denote $f_{\epsilon,h}$ its piecewise constant projection, then

$$\begin{aligned}
\|f - f_h\|_{\mathrm{L}^1} &\le \|f - f_\epsilon\|_{\mathrm{L}^1} + \|f_\epsilon - f_{\epsilon,h}\|_{\mathrm{L}^1} + \sum_{i=1}^{h} \epsilon_h \left| \fint_{x_{i-1}^h}^{x_i^h} (f - f_\epsilon) \,\mathrm{d}x \right| \\
&\le \|f - f_\epsilon\|_{\mathrm{L}^1} + \|f_\epsilon - f_{\epsilon,h}\|_{\mathrm{L}^1} + \sum_{i=1}^{h} \int_{x_{i-1}^h}^{x_i^h} |f - f_\epsilon| \,\mathrm{d}x \\
&\le 2\epsilon + \|f_\epsilon - f_{\epsilon,h}\|_{\mathrm{L}^1}.
\end{aligned}$$

Letting $h \to \infty$, we obtain $\lim_{h\to\infty} \|f - f_h\|_{\mathrm{L}^1} \le 2\epsilon$ for all $\epsilon > 0$. ■

Lemma 8 *There exists a constant c_2, depending only on $\|f\|_{\mathrm{L}^1}$ such that, for every $u \in \mathscr{A}$ with $E(u) < \infty$, the piecewise affine, continuous interpolants v_h of u with respect to the mesh (x_i^h) satisfy*

$$\|v_h - u\|_{\mathscr{A}} \to 0, E_h(v_h) \to E(u) \quad \text{as } h \to \infty,$$
$$\|v_h\|_{\mathscr{A}} \le 2\|u\|_{\mathscr{A}}, \text{ and } \quad E_h(v_h) \le \big[2\|f\|_{\mathrm{L}^1}^2 + \sup_{z\ge 1} J(z)\big] + E(u) + 2\|u\|_{\mathscr{A}}^2.$$

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

$$\int_{x_{i-1}^h}^{x_i^h} v_h' \,\mathrm{d}x = \int_{x_{i-1}^h}^{x_i^h} u' \,\mathrm{d}x,$$

and summing over i, we get $\|v_h'\|_{\mathrm{L}^2(0,1)} \le \|u'\|_{\mathrm{L}^2(0,1)}$. For $\|\cdot\|_{\mathscr{A}} = \|\cdot\|_{\mathrm{H}^1}$ only, we need to use Friedrich's inequality to obtain $\|v_h\|_{\mathscr{A}} \le 2\|u\|_{\mathscr{A}}$. It follows from standard interpolation error estimates and a simple density argument that

$$\|u - v_h\|_{\mathscr{A}} \to 0,$$

as $h \to \infty$.

To compute the bounds on the energy as well and to show its convergence, we start with the lower-order terms. Using Lemma 7 and the fact that $v_h(1) = u(1)$ for all $h \in \mathbf{N}$, we have

$$\begin{aligned} -\int_0^1 f_h v_h \,\mathrm{d}x - g v_h(1) &\to -\int_0^1 f u \,\mathrm{d}x - g u(1) \quad \text{as } h \to \infty, \text{ and} \\ -\int_0^1 f_h v_h \,\mathrm{d}x - g v_h(1) &\le -\int_0^1 f u \,\mathrm{d}x - g u(1) + 2\|f\|^2_{\mathrm{L}^2(0,1)} + 2\|u\|^2_{\mathscr{A}}, \end{aligned} \tag{3.5}$$

where we used

$$\begin{aligned} -\int_0^1 f_h v_h \,\mathrm{d}x &= -\int_0^1 f u \,\mathrm{d}x + \int_0^1 \left[f(u - v_h) + (f - f_h) v_h \right] \mathrm{d}x \\ &\le -\int_0^1 f u \,\mathrm{d}x + \|f\|_{\mathrm{L}^1} \|u - v_h\|_{\mathrm{L}^\infty} + \|f - f_h\|_{\mathrm{L}^1} \|v_h\|_{\mathrm{L}^\infty} \\ &\le -\int_0^1 f u \,\mathrm{d}x + 4\|f\|_{\mathrm{L}^1} \|u\|_{\mathscr{A}} \\ &\le -\int_0^1 f u \,\mathrm{d}x + 2\|f\|^2_{\mathrm{L}^1} + 2\|u\|^2_{\mathscr{A}}. \end{aligned}$$

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^h_{i-1}, x^h_i), we have $v'_h = h \int_{x^h_{i-1}}^{x^h_i} u' \,\mathrm{d}x$ and, using Jensen's inequality $J_0(v'_h) \le h \int_{x^h_{i-1}}^{x^h_i} J_0(u') \,\mathrm{d}x$ (note that $1/h$ is the length of the interval). If we define

$$a_h(x) = h \int_{x^h_{i-1}}^{x^h_i} J_0(u') \,\mathrm{d}x + \max_{z \ge 1} J(z), \qquad \text{for } x \in (x^h_{i-1}, x^h_i),$$

then $J(v'_h) \le a_h(x)$ a.e. in $(0,1)$ and

$$\int_0^1 a_h(x) \,\mathrm{d}x = \int_0^1 J_0(u') \,\mathrm{d}x + \max_{z \ge 1} J(z) =: A.$$

In particular, we also have

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

which, together with (3.5) gives

$$E_h(v_h) \le \left[2\|f\|^2_{\mathrm{L}^1} + \sup_{z \ge 1} J(z) \right] + E(u) + 2\|u\|^2_{\mathscr{A}}. \tag{3.6}$$

Since $x \mapsto J_0(u'(x)) \in \mathrm{L}^1(0,1)$, we have, by Lebesgue's differentiation theorem (Section 1.7, Corollary 2, [EG92])

$$\lim_{h \to \infty} a_h(x) = J_0(x) + \max_{z \ge 1} J(z)$$

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

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

$$\begin{aligned}
2A - \limsup_{h\to\infty} \int_0^1 \big|J(v_h') - J(u')\big|\,\mathrm{d}x &= \liminf_{h\to\infty} \int_0^1 \big[2a_h - |J(v_h') - J(u')|\big]\,\mathrm{d}x \\
&\geq \int_0^1 \liminf_{h\to\infty} \big[2a_h - |J(v_h') - J(u')|\big]\,\mathrm{d}x \\
&= 2\int_0^1 \big[J_0(u') + \max_{z\geq 1} J(z)\big]\,\mathrm{d}x \\
&= 2A,
\end{aligned}$$

and hence, using also (3.5), we have $E(v_h) \to E(u)$ as $h \to \infty$ ■

We have assembled all results to prove Theorem 5.

Proof of Theorem 5 The result is a straightforward application of Theorem 3, using the preparations of this Section.

Conditions (i) and (ii) were shown in Lemma 6. 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 8. Condition (v) is controlled by Lemma 7, since E_h and $E|_{\mathscr{A}_h}$ differ only in the forcing term.

Let $v_h(t)$ be the piecewise affine interpolant of $u(t)$. Using Lemma 8, to obtain (vi), we only need to show, that $t \mapsto v_h(t)$ 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 $\mathrm{C}[0,1]$, the mapping $t \mapsto u(t)$ lies in $\mathrm{C}(0,\infty;\mathrm{C}[0,1])$ and hence $t \mapsto u(x,t)$ is continuous as well. Since

$$v_h(x,t) = \sum_{j=1}^{h} u(x_j^h, t)\varphi_j^h(x),$$

where the φ_j^h are Lipschitz functions, this shows that $v \in \mathrm{C}(0,\infty;\mathrm{H}^1)$. ■

4 Convergence of local minimizers

4.1 Elastic deformation

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 [FT02] 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. In the present setting, where the potential $J(z)$ is bounded as $z \to \infty$, global minimization cannot give the correct answer, as the following proposition demonstrates.

Proposition 9 *Let E_h be the energy defined in* (3.1)*, with $f \equiv 0$ and $g \equiv 0$. For every $\epsilon > 0$, there exists an $H \in \mathbf{N}$ such that for all $h > H$, the global minimum of E_h among all orientation preserving deformations, satisfying $u(0) = 0, u(1) = 1 + \epsilon$ is not affine.*

Proof Consider the 'fractured' deformation $u_i^h = x_i^h$ for $i = 0, 1, \ldots, h-1$ and $u_h^h = 1 + \epsilon$. Then,

$$\begin{aligned} E_h((u_i^h)) &= \frac{h-1}{h} J(1) + \frac{1}{h} J(1 + \epsilon h) \\ &\leq \frac{h-1}{h} J(1) + \frac{1}{h} \sup_{z \geq 1} J(z), \end{aligned}$$

which, for sufficiently large h is strictly less than

$$E_h(((1+\epsilon)x_i^h)) = J(1+\epsilon) > J(1).$$

■

The proof actually showed that not only is the Cauchy-Born hypothesis violated, but in fact a material breaks for arbitrarily small boundary displacements or surface forces, if we assume that it attains the global energy minimum. On the other hand, one of the goals of this paper is to highlight the fact that for atomistic models, global minimization is the wrong approach. Proposition 9 only formalizes this.

In the following, we take a somewhat different version of the Cauchy-Born hypothesis, considering small forces rather than boundary displacements and showing that the resulting equilibria are essentially continua. The convergence result of Theorem 5 suggests the following procedure: For sufficiently small forces, there should be a critical point u_h^*, in fact a strict local minimum, of the atomistic functional E_h, such that $u_h^{*\prime} < z_1$, 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 u_h^* 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 u_h^*.

The main difficulty is to show that the critical points u_h^* are 'uniform local minimizers' in the sense that we do not require perturbations to tend to zero as $h \to \infty$. We formalize this in the following theorem.

Theorem 10 *Let E_h be the energy defined in* (3.1). *If $|g| + \|f\|_{\mathrm{L}^1} < J'(z_1)$, there exist critical points u_h^* of E_h in $\mathscr{A}_h$, such that $u_h^{*\prime} < z_1$. These equilibria are stable in the sense that any $|\cdot|_{\mathrm{H}^1}$-gradient flow u_h of E_h with $u_h'(0,x) < z_1$ satisfies $\lim_{t\to\infty} u_h(t) = u_h^*$ in $\mathrm{H}^1(0,1)$. There exists also $\tilde{\epsilon} > 0$ such that, if u_h is an $\|\cdot\|_{\mathrm{H}^1}$- gradient flow with $u_h'(0,x) \le u_h^{*\prime}(x) + \tilde{\epsilon}$, then we have $u_h(t) \to u_h^*$ as $t \to \infty$ as well.*

Furthermore, there exists a critical point $u^* \in \mathscr{A}$ of E such that $\lim_{h\to\infty} u_h^* = u^*$ and $\lim_{t\to\infty} u(t) = u^*$ in H^1, for every $|\cdot|_{\mathrm{H}^1}$- gradient flow u of E with $u'(0,x) \le z_1 - \epsilon$ for some $\epsilon > 0$, and for every $\|\cdot\|_{\mathrm{H}^1}$-gradient flow u of E with $u'(0,x) \le u^{*\prime}(x) + \tilde{\epsilon}$.

If $f \equiv 0$, then $u_h^* = u^*$ are affine.

This result has two interpretations. First, we may interpret it as some form of the Cauchy-Born hypothesis, i.e., that the atomistic deformation is essentially a continuum deformation. Second, it shows that the resulting continuum model has the correct behaviour for small loads.

Note also, that not all proofs in this Section are 'optimal'. Especially the proof of Theorem 10 is more technical than it needs to be. The purpose of this discussion is to show that some of the techniques used here can be applied to far more general problems and are in particular dimension independent.

The proof of Theorem 10 requires some preparation in the form of several Lemmas which assemble information about the atomistic gradient flow.

We 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 11 *Suppose that $|g| + \|f\|_{\mathrm{L}^1(0,1)} \le J'(z_1 - \epsilon)$ for some $\epsilon > 0$; then there exists a unique critical point u_h^* of E_h in the set $\mathscr{B}_\epsilon$. The point u_h^* satisfies*

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

where F_j^h is defined by (4.3).

Proof We compute the critical point by a change of variables. For $u_h \in \mathscr{A}_h$, let $r_j^h = (u_j^h - u_{j-1}^h)/\epsilon_h$. Then, setting

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

we have, using $u_0^h = 0$,

$$\begin{aligned} E_h(u_h) &= \sum_{j=1}^h \epsilon_h J(r_j^h)) - \sum_{j=0}^h \epsilon_h \tilde f_j^h u_j^h - g u_h^h \\ &= \sum_{j=1}^h \epsilon_h J(r_j^h)) - \sum_{j=1}^h \epsilon_h \tilde f_j^h \sum_{i=1}^j \epsilon_h r_i^h \\ &= \sum_{j=1}^h \epsilon_h J(r_j^h)) - \sum_{i=1}^h \epsilon_h r_i^h \Big[g + \sum_{j=i}^h \epsilon_h \tilde f_j^h \Big] \\ &= \sum_{j=1}^h \epsilon_h \big[J(r_j^h) - F_j^h r_j^h \big], \end{aligned}$$

where

$$F_i^h = g + \sum_{j=i}^h \epsilon_h \tilde f_j^h = g + \frac{\epsilon_h}{2}(f_i^h + f_h^h) + \sum_{j=i+1}^{h-1} \epsilon_h f_j^h. \tag{4.3}$$

To compute r_j^h, we differentiate E_h with respect to r_j^h, which gives the equation

$$\frac{\partial E_h(u_h)}{\partial r_j^h} = \epsilon_h \big[J'(r_j^h) - F_j^h \big] = 0 \quad \text{for } j = 1, \ldots, h,$$

or, equivalently,

$$J'(r_j^h) = F_j^h.$$

We estimate F_j^h, using the assumption that $\|f\|_{\mathrm{L}^1} + g \le J'(z_1 - \epsilon)$, by

$$\begin{aligned} |F_j^h| &= \left| g + \frac{1}{2} \int_{x_{j-1}^h}^{x_j^h} f(x)\,\mathrm{d}x + \int_{x_j^h}^{x_{h-1}^h} f(x)\,\mathrm{d}x + \frac{1}{2} \int_{x_{h-1}^h}^1 f(x)\,\mathrm{d}x \right| && (4.4) \\ &\le |g| + \int_{x_{j-1}^h}^1 |f(x)|\,\mathrm{d}x \\ &\le |g| + \|f\|_{\mathrm{L}^1(0,1)} && (4.5) \\ &\le J'(z_1 - \epsilon). && (4.6) \end{aligned}$$

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

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

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

Lemma 12 *Under the conditions of Lemma 11, if $u_h : [0,\infty) \to \mathscr{A}_h$ is an $|\cdot|_{\mathrm{H}^1}$-gradient flow of E_h with $u_h(0) \in \mathscr{B}_\epsilon$ then $u_h(t) \in \mathscr{B}_\epsilon$ for all $t > 0$.*

Proof Consider the time-discrete approximation $(U_h(t_j))_{j=0,1,\ldots}$, as described in Lemma 4, for some fixed, sufficiently small time-step τ. Let $R_h^i(t_j)$ be as in the proof of Lemma 11. Then, $R_h(t_j)$ minimizes

$$\frac{1}{2\tau}\|R_h(t_j) - R_h(t_{j-1})\|_{L^2}^2 + E_h(R_h(t_j)). \tag{4.7}$$

As in the proof of Lemma 11, we compute the Euler–Lagrange equation in terms of $R_h^i(t_j)$. At the minimum, the equation

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

has to be satisfied. For sufficiently small τ, there is a unique solution. Now assume (inductively) that $R_h^i(t_{j-1}) \le z_1 - \epsilon$. To show that $R_h^i(t_j) \le z_1 - \epsilon$, assume this is not true. Then $F_j^h - J'(R_h^i(t_j)) < 0$, which gives a contradiction. Hence, we have that for all $i = 1, \ldots, h$ and $j \in \mathbf{N}$,

$$R_h^i(t_j) \le z_1 - \epsilon.$$

As $\tau \to 0$, the discrete solution converges to the gradient flow u_h and hence $u_h' \le z_1 - \epsilon$ a.e. in $(0,1)$. ■

Corollary 12A *Under the conditions of Lemma 11, every $|\cdot|_{\mathrm{H}^1}$-gradient flow u_h with $u_h(0) \in \mathscr{B}_\epsilon$ satisfies the evolutionary variational inequality*

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}|u_h - v|_{\mathrm{H}^1}^2 + \frac{\alpha}{2}|u_h - v|_{\mathrm{H}^1}^2 + E_h(u_h) \le E_h(v) \quad \forall v \in \mathscr{B}_\epsilon, \tag{4.8}$$

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

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

Proof We set $\tilde{E}_h = E_h|_{\mathscr{B}_\epsilon}$ and show that u_h is also a gradient flow for $\tilde{E}_h$ by considering the minimization problem (4.7) again. Since the minimizer remains in $\mathscr{B}_\epsilon$, it is also the minimizer of

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

and hence the limit of the time-discretizations must also be the gradient flow of $\tilde{E}_h$. By arguing as in the proof of Lemma 6, we find that $\tilde{E}_h$ is α-convex (i.e. λ-convex with $\lambda = \alpha$), and hence u_h satisfies (4.8) for all v if we replace E_h with $\tilde{E}_h$. For $v \in \mathscr{B}_\epsilon$, however, the functionals are the same, and hence (4.8) holds for all $v \in \mathscr{B}_\epsilon$.

On testing (4.8) with $v = u_h^*$, and multiplying the resulting inequality by $e^{2\alpha t}$, we obtain

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

Integrating from 0 to T gives the result. ■

For the H^1-norm gradient flow, we have slightly weaker results, as it is more difficult to say when the gradient decays.

Lemma 13 *Let $\|f\|_{\mathrm{L}^1} + |g| < J'(z_1)$ and suppose that u_h is an $\|\cdot\|_{\mathrm{H}^1}$-gradient flow of E_h with initial condition satisfying*

$$J'(u_h'(0,x)) \leq F_i^h + \delta \quad \text{for } x \in (x_{i-1}^h, x_i^h), \text{ for } i = 1, \dots, h, \tag{4.9}$$

where $\delta > 0$ is such that $\|f\|_{\mathrm{L}^1} + |g| + \delta < J'(z_1)$, for $i = 1, \dots, h$. Then,

$$J'(u_h'(t,x)) \leq F_i^h + \delta \ \text{ for } t > 0,\ x \in (x_{i-1}^h, x_i^h), \text{ and } i = 1, \dots, h.$$

In particular, u_h satisfies

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|u_h(t) - v\|_{\mathrm{H}^1}^2 + \frac{\alpha}{2}\|u_h(t) - v\|_{\mathrm{H}^1}^2 + E_h(u_h) \leq E_h(v) \quad \forall v \in \mathscr{B}_\epsilon,$$

where $\alpha = \min\{J''(z) : 0 < z \leq \|f\|_{\mathrm{L}^1} + |g| + \delta\}$, and we have

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

Proof We consider again the implicit time-discretization of the gradient flow $(U_h(t_j))_{j=0,2,\dots} \subset \mathscr{A}_h$, so that

$$U_h(t_j) \text{ minimizes } \frac{\|\cdot - U_h(t_{j-1})\|_{\mathrm{H}^1}^2}{2\tau} + E_h(\cdot). \tag{4.10}$$

The quadratic terms can be rewritten in terms of matrix-vector products. Let I_h be the $h \times h$ identity matrix, $M = (M_{ij}) \in \mathbf{R}^{h\times h}$ be the mass matrix, i.e., the symmetric tridiagonal matrix

$$M = \frac{1}{6}\begin{bmatrix} 4 & 1 & & & \\ 1 & 4 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & 4 & 1 \\ & & & 1 & 4 \end{bmatrix}.$$

Let $W = (W_i)_{i=1,\dots,h}$ be the vector of nodal values of a piecewise affine function w_h at $x_1^h, \dots, x_h^h$, then

$$\|w_h\|_{\mathrm{L}^2}^2 = \frac{1}{h}W^\top M W.$$

Let $Q = (Q_i)_{i=1,\dots,h}$, $Q_i = h(W_i - W_{i-1})$ (letting $W_0 = 0$), then

$$W = SQ,$$

where $S = (S_{ij}) \in \mathbf{R}^{h\times h}$ is the lower triagonal matrix with $S_{ij} = 1/h$ for $i \leq j$,

$$S = \frac{1}{h}\begin{bmatrix} 1 & & \\ \vdots & \ddots & \\ 1 & \dots & 1 \end{bmatrix}.$$

This gives us

$$\|w_h\|_{\mathrm{L}^2}^2 = \frac{1}{h}Q^\top S^\top M S Q \ \text{ and } \ \|w_h'\|_{\mathrm{L}^2}^2 = \frac{1}{h}Q^\top I_h Q.$$

Upon setting $R_h^i(t_j) = U_h'(t_j)$ in (x_{i-1}^h, x_i^h), we can therefore write

$$\|U_h(t_j) - U_h(t_{j-1})\|_{\mathrm{H}^1}^2 = \frac{1}{h}[R_h(t_j) - R_h(t_{j-1})]^\top \Big(I_h + S^\top MS\Big)[R_h(t_j) - R_h(t_{j-1})],$$

and the minimization problem (4.10) becomes

$$\Big(I_h + S^\top MS\Big)\frac{R_h(t_j) - R_h(t_{j-1})}{\tau} = G(t_j), \tag{4.11}$$

where $G_i(t_j) = F_i^h - J'(R_h^i(t_j))$.

Denote $A = (I_h + S^\top MS)^{-1}$. It follows from Lemma 14 below that $A = (A_{ij})$ satisfies $A_{i,j} < 0$ if $i \neq j$, and it is strictly row diagonally dominant, i.e.,

$$A_{ii} > -\sum_{j\neq i} A_{i,j} \quad \text{for } i = 1, \dots, h.$$

Since we are in finite dimensions, we can strengthen this to

$$A_{ii} > -\rho\sum_{j\neq i} A_{i,j} \quad \text{for } i = 1, \dots, h, \tag{4.12}$$

where $\rho > 1$ may depend on h.

In terms of the G_i, the condition (4.9), we have placed on the initial configuration, may be translated into $G_k(0) \geq -\delta$. We claim that $G_k(t_j) \geq -\delta$ for all $j \in \mathbf{N}, k = 1, \dots, h$. Suppose that this holds at time t_{j-1}, and, for contradiction, suppose that

$$G_k(t_j) < -\delta \;\text{ and }\; G_i(t_j) \geq -\rho\delta \quad \text{for } i = 1, \dots, h. \tag{4.13}$$

By choosing τ sufficiently small, we can always achieve this: using norm-equivalence, we have $F \in \ell^\infty$, which can be used to infer from (4.11) that $R_h^i(t_j) \geq \beta > 0$, for all i and j. Hence, $J'(R_h^i(t_j))$ remains bounded, which implies that $\|G(t_j)\|_{\ell^\infty} \leq C_1$ for all j. This, in turn, gives $\|R_h(t_j) - R_h(t_{j-1})\|_{\ell^\infty} \leq \tau\|A\|_{\ell^\infty}C_1$.

From (4.12) and (4.13), we have

$$\begin{aligned}(AG(t_j))_k &= a_{kk}G_k(t_j) + \sum_{i\neq k} a_{ik}G_i(t_j)\\ &< -a_{kk}\delta - \rho\delta\sum_{i\in I_k} a_{ik}\\ &< 0.\end{aligned}$$

Hence, by (4.11), $R_h^k(t_j) < R_h^k(t_{j-1})$, or equivalently, $G_k(t_j) > G_k(t_{j-1})$, which contradicts our assumption that $G_k(t_{j-1}) \geq -\delta$ and $G_k(t_j) < -\delta$. Hence, we have established that $G_i(t_j) \leq \delta$ for all $i = 1, \dots, h$ and $j \in \mathbf{N}$. Letting $\tau \to 0$, we obtain

$$J'(u_h'(t,x)) \leq F_h^i + \delta \quad \text{for } x \in (x_{i-1}^h, x_i^h) \text{ and } t \geq 0.$$

The variational inequality and the exponential convergence to the critical point follow exactly as in the proof of Corollary 12A. ■

Lemma 14 *Let $A = (A_{i,j}) = (I_h + S^\top MS)^{-1}$ be the matrix defined in the proof of Lemma 13. Then A satisfies $A_{i,j} < 0$ for $i \neq j$ and it is strictly row diagonally dominant, i.e.,*

$$A_{ii} > -\sum_{j\neq i} A_{i,j}.$$

The proof of Lemma 14 is given in Appendix A. Before we start the proof of Theorem 10, we formulate a minor technical lemma.

Lemma 15 *Let $f \in \mathrm{L}^1(0,1)$, then*

$$\max_{i=1,\ldots,h} \int_{x_{i-1}^h}^{x_i^h} |f| \, \mathrm{d}x \to 0 \text{ as } h \to \infty,$$

where $x_i^h = ih$, for $h \in \mathbf{N}$, and $i = 0, 1, \ldots, h$.

Proof To prove this, let χ_h be the characteristic function of the interval where the maximum is attained, and, for any given $\epsilon > 0$, fix $M > 0$ such that

$$\int_0^1 \big[|f| - \min(M, |f|)\big] \, \mathrm{d}x \leq \epsilon.$$

We have

$$\begin{aligned} \int_0^1 \chi_h |f| \, \mathrm{d}x &= \int_0^1 \chi_h(|f| - \min(M,|f|)) \, \mathrm{d}x + \int_0^1 \chi_h \min(M,|f|) \, \mathrm{d}x \\ &\leq \epsilon + \frac{M}{h} \to \epsilon \quad \text{as } h \to \infty. \end{aligned}$$

Since ϵ was an arbitrary positive number, we have the result. ∎

Proof of Theorem 10 After Lemmas 11, 12, 12A, and 13 we only need to establish the facts about the continuum limit. We can treat both gradient flows simultaneously.

Note that most of the following analysis is independent of the specific structure of the problem. All we require below, is that $u_h(t) \to u(t)$ as $h \to \infty$, for every $t \geq 0$, and $u_h(t) \to u_h^*$ as $t \to \infty$, uniformly in h. In order to achieve this we only need to show that given an initial condition $u(0)$ for the 'continuum' $\mathscr{A}$-gradient flow satisfying the assumptions of the theorem, there exist 'discrete' initial conditions $u_h(0)$ which satisfy the assumptions of Lemma 12 or 13.

Let $u'(0,x) \leq z_1 - \epsilon$ for a.e. $x \in (0,1)$. Letting $u_h(0,x)$ be the piecewise affine interpolant of $u'(0,x)$, we have

$$u_h'(0,x) = \frac{1}{\epsilon_h} \int_{x_{i-1}^h}^{x_i^h} u'(0,x) \, \mathrm{d}x \leq z_1 - \epsilon,$$

if $u'(0,x) \leq z_1 - \epsilon$ (the condition for the $|\cdot|_{\mathrm{H}^1}$-gradient flow).

The condition on the initial data for the $\|\cdot\|_{\mathrm{H}^1}$-gradient flow is slightly more difficult to verify. Given an initial condition $u(0,x)$ satisfying $J'(u'(0,x)) \leq J'(u^{*\prime}(x)) + \delta$, we shall find an atomistic initial condition $u_h(0,x)$ such that for arbitrarily small δ_1, we have

$$J'(u_h'(0,x)) \leq J'(u_h^{*\prime}(x)) + \delta + \delta_1, \tag{4.14}$$

when h is sufficiently large. As usual, we take the piecewise affine interpolant of $u(0,x)$ and we have for $x \in (x_{i-1}^h, x_i^h)$ and for some point $\xi_i^h \in (x_{i-1}^h, x_i^h)$,

$$\begin{aligned} J'(u_h'(0,x)) &\leq J'(u'(0,\xi_i^h)) \\ &\leq \int_{\xi_i^h}^1 f(x)\,\mathrm{d}x + g + \delta \\ &\leq F_i^h + \delta + \left| \int_{\xi_i^h} f\mathrm{d}x - \int_{x_i^h}^1 f\mathrm{d}x - \frac{1}{2}\int_{x_{i-1}^h}^{x_i^h} f\mathrm{d}x + \frac{1}{2}\int_{x_{h-1}^h}^{x_h^h} f\mathrm{d}x \right| \\ &\leq F_i^h + \delta + \frac{1}{2}\int_{x_{i-1}^h}^{x_i^h} |f|\mathrm{d}x + \frac{1}{2}\int_{x_{h-1}^h}^{x_h^h} |f|\mathrm{d}x. \end{aligned}$$

To prove that $u_h'(0,x)$ satisfies (4.14) for sufficiently large h, we require that

$$\max_{i=1,\dots,h} \int_{x_{i-1}^h}^{x_i^h} |f|\,\mathrm{d}x \to 0 \text{ as } h \to \infty,$$

which is shown in Lemma 15.

Therefore, the atomistic $\mathscr{A}$-gradient flows with starting point $u_h'(0,\cdot)$ converge exponentially with exponent α independent of h (compare Corollary 12A and Lemma 13) to the equilibrium u_h^*. We use this fact to estimate

$$\begin{aligned} \|u_h^* - u_k^*\|_{\mathscr{A}} &\leq \|u_h^* - u_h(t)\|_{\mathscr{A}} + \|u_h(t) - u_k(t)\|_{\mathscr{A}} + \|u_k(t) - u_k^*\|_{\mathscr{A}} \\ &\leq 2e^{-\alpha t} + \|u_h(t) - u_k(t)\|_{\mathscr{A}}, \end{aligned}$$

thus showing that $(u_h^*)_{h\in\mathbf{N}}$ is a Cauchy-sequence. We denote its limit by u^*. To see that $u(t) \to u^*$ as $t \to \infty$, consider

$$\begin{aligned} \|u(t) - u^*\|_{\mathscr{A}} &\leq \inf_{h\in\mathbf{N}} (\|u(t) - u_h(t)\|_{\mathscr{A}} + \|u_h(t) - u_h^*\|_{\mathscr{A}} + \|u_h^* - u^*\|) \\ &\leq e^{-\alpha t}. \end{aligned}$$

We have shown that the 'discrete' equilibria u_h^* converge to a 'continuum' deformation u^* and that $u(t) \to u^*$.

The fact that u^* is a critical point of E follows from the general theory as well. It is straightforward to show that the functionals E_h Γ-converge to E in the strong H^1 topology. Since they are also uniformly λ-convex, Proposition 13 in [Ort05], a liminf inequality for the slopes, shows that

$$|\partial E|(u^*) \leq \liminf_{h\to\infty} |\partial E_h|(u_h^*) = 0,$$

where $|\partial\phi|(u)$ denotes the local slope of a functional ϕ at u,

$$|\partial\phi|(u) = \limsup_{v\to u} \frac{(\phi(u) - \phi(v))^+}{\|u - v\|_{\mathscr{A}}}.$$

To establish the Γ-convergence, note that Lemma 8 gives the limsup condition. For the liminf condition, we write

$$E_h(u_h) = \phi(u_h) + C_h(u_h), \;\; E(u) = \phi(u) + C(u),$$

where

$$\begin{aligned}
\phi(u) &= \int_0^1 J_0(u')\,\mathrm{d}x \\
C_h(u_h) &= \int_0^1 J_1(u_h') - f_h u_h\,\mathrm{d}x - g u_h(1) \\
C(u) &= \int_0^1 J_1(u') - f u\,\mathrm{d}x - g u(1).
\end{aligned}$$

Hence, $C_h(u_h) \to C(u)$, whenever u_h is piecewise affine and $u_h \to u$ in H^1. Setting $C_h(u) = \infty$ if u is not piecewise affine, we get $\liminf_h C_h(u_h) \geq C(u)$, whenever $u_h \to u$. Since ϕ is convex, it is lower semicontinuous by standard results, and hence E_h $\Gamma(\mathrm{H}^1)$-converges to E. ∎

4.2 A (counter-) example

In this section, we consider again the situation of Theorem 10, and construct an H^1-continuous curve $u(s)$ such that $u(0) = u^*$ is the elastic equilibrium computed in the previous Section, and which satisfies $E(u(s)) < E(u(0))$ for $s > 0$, thus showing that the limit of the gradient flow is in fact not a local minimum of E with respect to the H^1 topology.

We consider the continuum limit energy, neglecting the body force,

$$E(u) = \int_0^1 J(u')\,\mathrm{d}x - g u(1), \tag{4.15}$$

where g is positive but small, so that Theorem 10 applies. We use $\mathrm{C}^{0,\alpha}$ to denote the space of Hölder continuous mappings.

Proposition 16 *Let u^* be the elastic equilibrium of E, described by Theorem 10. If $0 < g < J'(z_1)$ and $f \equiv 0$, then there exists $s_0 > 0$ such that, for every $1 \leq p < \infty$, there exists a curve $u \in \mathrm{C}^{0,1/p}(0, s_0; \mathrm{W}^{1,p}(0,1))$, $u(0) = u^*$ such that $E(u(s)) < E(u^*)$ for $0 < s \leq s_0$. In particular, in the case $p = 1$, u is Lipschitz continuous in $\mathrm{W}^{1,1}$.*

Proof Define the $\mathrm{W}^{1,\infty}$-perturbation $u(s) \in \mathscr{A}$ of u^* by

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

Then, letting $J_\infty = \sup_{z \geq 1} J(z)$, we have for for $s < g/(J(u^{*\prime}) - J_\infty)$,

$$\begin{aligned}
E(u^*) - E(u(s)) &= J(u^{*\prime}) - g u^{*\prime} - (1 - s^k) J(u^{*\prime}) - s^k J_\infty + g u^{*\prime} + s^{k-1}) \\
&= s^k (J(u^{*\prime}) - J_\infty) - g s^{k-1} \\
&> 0.
\end{aligned}$$

Furthermore, we have for $0 < s < t$,

$$\begin{aligned} \|u'(t) - u'(s)\|_{\mathrm{L}^p}^p &= s^k \left(\frac{1}{s} - \frac{1}{t}\right)^p + (t^k - s^k)\frac{1}{t^p} \\ &\leq \frac{s^k}{(ts)^p}(t-s)^p + \frac{kt^{k-1}}{t^p}(t-s) \\ &\leq C(t-s), \end{aligned}$$

if $k \geq 2p \geq 2$. For $0 < s$, we have

$$\|u'(s) - u'(0)\|_{\mathrm{L}^p}^p = s^k \frac{1}{s^p} \leq C(s-0),$$

if $k \geq p+1$. Thus, under the given hypothesis, we have that $u \in \mathrm{C}^{0,1/p}(0, s_0; \mathrm{W}^{1,p}(0,1))$, and in particular, that it is Lipschitz-continuous in $\mathrm{W}^{1,1}(0,1)$. ■

Why, we should ask ourselves, is Proposition 4.2 not in contradiction with Theorem 10? If there exists a curve along which the energy decreases, should the gradient flow not find this curve? The explanation is that the curve $u(s)$ which we have constructed is not Lipschitz continuous in $\mathrm{H}^1(0,1)$ and hence is not a candidate for the gradient flow evolution. A slightly refined analysis would in fact reveal that $s \mapsto u(s)$ is not even absolutely continuous in H^1, as the finite differences $(u(t) - u(s))/(t-s)$ do not converge in the H^1-norm as $t \to s$.

An interesting question is, whether there actually can exist an absolutely continuous curve starting in u^*, 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. In the following Proposition, we provide another example, which suggests that it is indeed unlikely that smooth curves leading out of the elastic equilibrium exist along which the energy decreases.

Proposition 17 *Let u^* be the elastic equilibrium from Theorem 10 where $f \equiv 0$ and $g < J'(z_1)$. Suppose that $v \in \mathscr{A}$, and define $u(s) = u^* + sv$. Then, $E(u(s)) > E(u^*)$ for all $s > 0$.*

Proof Note first, that the equilibrium u^* satisfies $J'(u^{*\prime}(x)) = g$ for all $x \in (0,1)$. We can write the difference $E(u(s)) - E(u^*)$ as

$$\begin{aligned} E(u(s)) - E(u^*) &= \int_0^1 \left[J(u^{*\prime} + sv') - J(u^{*\prime})\right] \mathrm{d}x - g(u^*(1) + sv(1)) + gu^*(1) \\ &= \int_0^1 \int_0^s J'(u^{*\prime} + tv')v' \,\mathrm{d}t \,\mathrm{d}x - sgv(1). \end{aligned}$$

If $v' < 0$, then $J'(u^{*\prime} + tv') < J'(u^{*\prime}) = g$, using the convexity of J in $(-\infty, z_1)$, and hence $J'(u^{*\prime} + tv')v' > gv'$. Similarly, if $v' > 0$, we have $J'(u^{*\prime} + tv')v' > gv'$ again.

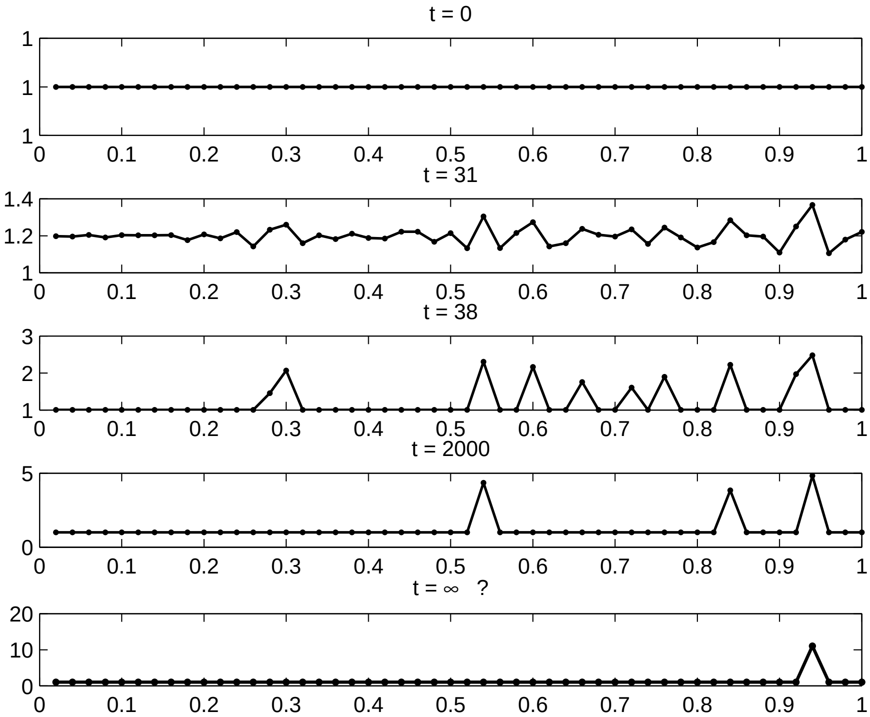

Figure 1: Snapshots of the deformation gradients of an $|\cdot|_{H^1}$-gradient flow evolution, showing the instability of the final state, computed with 51 'atoms'. The new final state ($t = \infty$) after instability sets in is not computed but guessed. This figure shows an *unstable* computation and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

Hence, we conclude that

$$E(u(s)) - E(u^*) \; > \; \int_0^1 \int_0^s gv' \,\mathrm{d}t\mathrm{d}x - sgv(1) \; = \; sg(v(1) - v(0)) - sgv(1) \; = \; 0.$$

∎

Finally, let us also remark that Proposition 16 shows that we could not have used a much weaker topology for the gradient flow. For example, the equilibrium u^* would be highly unstable under arbitrary perturbations, with respect to the L^2-gradient flow (leaving aside for the moment, that we do not even have an existence theory for such an evolution).

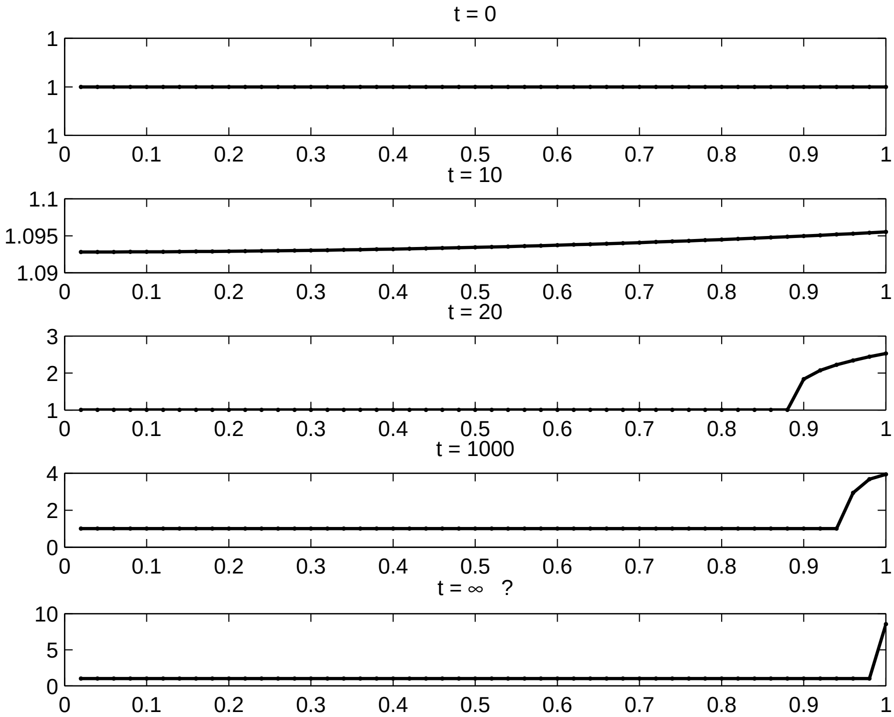

Figure 2: Snapshots of the deformation gradients of an $\|\cdot\|_{H^1}$-gradient flow evolution, converging to a 'surface fracture' state, computed with 51 'atoms'. The final state is not computed but guessed. Note also the different scales in the respective plots.

4.3 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. If we do not restrict the motion of the material further, i.e., if we let $M = \infty$, then the gradient flows $u_h(t)$ and $u(t)$ 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, $z_1 < M < \infty$.

In this Section, we demonstrate another interesting, but possibly slightly worrying property of gradient flow evolutions. We show that the results may change significantly, if we change the norm in which we consider the gradient flow, but we do it in such a way that the topology remains the same. Since the problem becomes analytically too complicated, much of the experience gained here will be based on numerical experiments. Note that the convergence result of Theorem 5

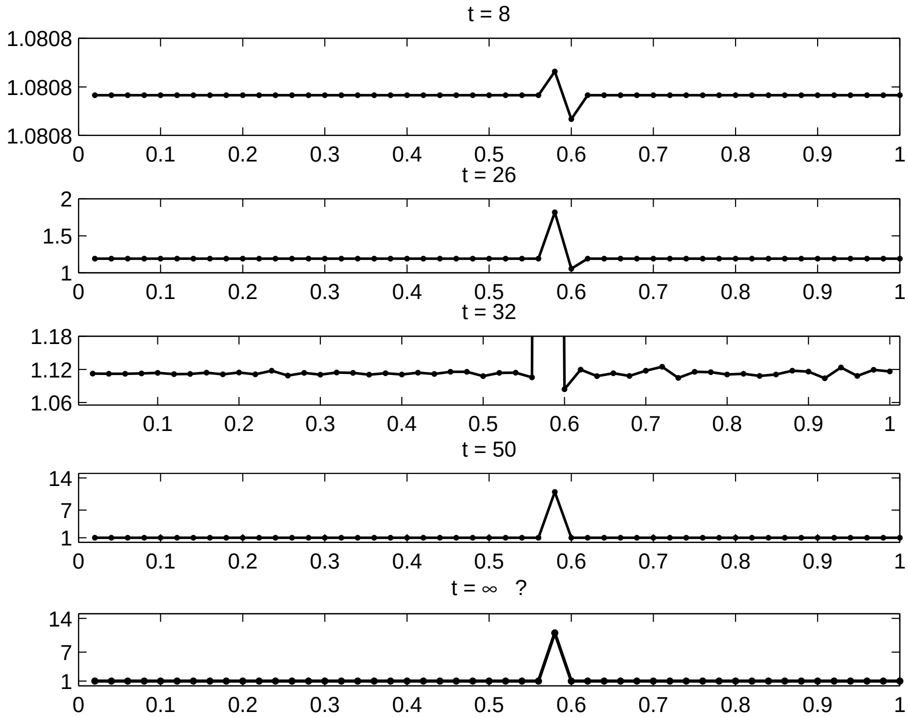

Figure 3: Snapshots of the deformation gradients of an $|\cdot|_{H^1}$-gradient flow evolution, computed with 51 'atoms', with a controlled perturbation at time $t = 7.6$ by an amount of 10^{-8}. The final state ($t = \infty$) after instability sets in is not computed but guessed. Note also the different scales in the respective plots.

represents also a convergence result for the numerical method.

For simplicity, we assume throughout this section that $f \equiv 0$ and $g > J'(z_1)$.

Proposition 18 *The solution of the $|\cdot|_{H^1}$-gradient flow in $\mathscr{A}$ with $u(0,x) = x$ is*

$$u(t,x) = \alpha(t)x,$$

where $\alpha(t)$ is strictly increasing until $u(t,1) = M$ and then remains constant.

Proof We change coordinates to $r(t,x) = u'(t,x)$, 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 $u(t_1, 1) = M$, the deformation u will be fixed at $u(1, t) = M$ for $t \geq t_1$. To see this, suppose that $u(t_1 + \tau_1, 1) < M$. Then, there exists a $\tau_2 < \tau_1$ such that $u(t_1 + \tau_1, 1) < u(t_1 + \tau_2, 1) < M$ as well. In this case, however, the above argument applies, and we have $r_t(t, x) \geq 0$ until $u(t, 1) = M$ again. We conclude that $u(t, 1) = M$ for all $t > t_1$.

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

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

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

The analytical solution obtained above is highly unstable under perturbation, as Figure 1, where a numerical computation is shown, demonstrates. In all computations, we chose J such that $z_2 = +\infty$, i.e., there exists no threshold for the deformation gradient beyond which there are no internal forces.

Changing the norm with respect to which we consider the gradient flow to the full H^1-norm gives a very different evolution, as can be seen in Figure 2. This evolution seems to be far more stable, as the results can be accurately reproduced when changing the mesh or the time-steps.

We perform one last experiment, in which we dominate the numerical round-off errors, and thus the instabilities in the $|\cdot|_{\mathrm{H}^1}$-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 3 for the computational results. If we perform the same experiment for the $\|\cdot\|_{\mathrm{H}^1}$-gradient flow, the final result does not change, which is another strong indication for the superior stability of this evolution.

Remark 19 *The unstable evolution may actually be preferred in practice, as it could be thought of representing the uncertainty of where damage occurs better. Unless specific defects are known, it is usually impossible to predict exactly where fracture occurs.*

A Proof of Lemma 14

We review briefly how the matrix A, which is the topic of this appendix is defined. Let M be the 'mass matrix'

$$M = \frac{1}{6}\begin{bmatrix} 4 & 1 & & & \\ 1 & 4 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & 4 & 1 \\ & & & 1 & 0 \end{bmatrix},$$

and S the 'antiderivative matrix'

$$S = \frac{1}{h}\begin{bmatrix} 1 & & \\ \vdots & \ddots & \\ 1 & \dots & 1 \end{bmatrix},$$

then A is defined as

$$A = (I + S^\top MS)^{-1},$$

which we can also rewrite in the more useful form

$$A = (I + S^\top MS)^{-1} = S^{-1}(S^{-\top}S^{-1} + M)^{-1}S^{-\top}.$$

The matrix S^{-1} is the 'difference operator'

$$S^{-1} = h\begin{bmatrix} 1 & & & & \\ -1 & 1 & & & \\ & -1 & 1 & & \\ & & \ddots & \ddots & \\ & & & -1 & 1 \end{bmatrix},$$

and its product with $S^{-\top}$ is the 'centered second difference operator'

$$S^{-\top}S^{-1} = h^2\begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 1 \end{bmatrix}.$$

Set $B = S^{-\top}S^{-1} + M$, then,

$$B = \frac{1}{6}\begin{bmatrix} 12h^2+4 & -6h^2+1 & & & \\ -6h^2+1 & 12h^2+4 & -6h^2+1 & & \\ & \ddots & \ddots & \ddots & \\ & & -6h^2+1 & 12h^2+4 & -6h^2+1 \\ & & & -6h^2+1 & 6h^2+4 \end{bmatrix}.$$

Denote $a = 2h^2+4/6$, $\tilde{a} = h^2+4/6$, $b = h^2-1/6$. Gaussian elimination, performed by hand, determines $D = B^{-1}$ by a set of recursive formulae. The elimination process can be performed in two ways. If we eliminate the subdiagonal first, we obtain in particular the relations

$$\begin{aligned} c_1 &= a, \ c_{i+1} = a - \frac{b^2}{c_i} \quad \text{for } i = 1, \ldots, h-2, \ c_h = \tilde{a} - \frac{b^2}{c_{h-1}}, \\ d_{i,j} &= \frac{b}{c_i} d_{i+1,j} \quad \text{for } i = h-1, \ldots, 1; j = i+1, \ldots, h. \end{aligned} \tag{A.16}$$

If we eliminate the superdiagonal first, then the counterparts of (A.16) are

$$\begin{aligned} c'_1 &= \tilde{a}, \quad c'_{i+1} = a - \frac{b^2}{c_i} \quad \text{for } i = 1, \ldots, h-1, \\ d_{i,j} &= \frac{b}{c'_i} d_{i-1,j} \quad \text{for } i = 2, \ldots, h; j = 1, \ldots, i-1. \end{aligned} \tag{A.17}$$

Both relations for the entries of D will be used below. Note also, that we have $d_{i,j} = d_{j,i}$, as B is symmetric. We collect some useful information about the matrix D in the following lemma.

Lemma 20 *The numbers c_i, c'_i defined above satisfy*

$$\begin{aligned} c_i &> \frac{i+1}{i} b \text{ for } i = 1, \ldots, h-1; \quad c_h > \frac{1}{h+1} b, \\ c'_i &> b \quad \text{for } \ i = 1, \ldots, h. \end{aligned} \tag{A.18}$$

and the $d_{i,j}$ satisfy

$$\begin{aligned} d_{i+1,j} &< d_{i,j} \quad \text{for } j = 1, \ldots, h-1; i = j, \ldots, h-1, \\ d_{i,j+1} &> d_{i,j} \quad \text{for } i = 2, \ldots, h; j = 1, \ldots, i-1. \end{aligned} \tag{A.19}$$

Proof First, note that $c_1 = a > 2b$, hence (A.18) holds for $i = 1$. Suppose, inductively, that (A.18) holds for some $i \leq h-2$. Then,

$$c_{i+1} = a - \frac{b^2}{c_i} > 2b - \frac{i}{i+1} b = \frac{i+2}{i+1} b,$$

which proves (A.18) for $i = 1, \ldots, h-1$. For c_h, we have that

$$c_h = \tilde{a} - \frac{b^2}{c_{h-1}} > b - \frac{h}{h+1} b = \frac{1}{h+1} b.$$

The proof for the c'_{i+1} follows along the same lines. First, $c'_1 = \tilde{a} > b$, and second, if $c'_i > b$, then

$$c'_{i+1} = a - \frac{b^2}{c'_i} > 2b - b = b.$$

To prove the bounds on the entries of D, we use

$$d_{i+1,j} = \frac{b}{c'_{i+1}} d_{i,j} < d_{i,j},$$

and

$$d_{i,j} = d_{j,i} = \frac{b}{c_j} d_{j+1,i} < d_{j+1,i} = d_{i,j+1}.$$

■

We compute $A = (I + S^\top MS)^{-1} = S^{-1}DS^{-\top}$, giving

$$A = h^2 \begin{bmatrix} d_{1,1} & d_{1,2} - d_{1,1} & d_{1,3} - d_{1,2} & \cdots \\ d_{2,1} - d_{1,1} & d_{1,1} + d_{2,2} - d_{1,2} - d_{2,1} & d_{1,2} + d_{2,3} - d_{1,3} - d_{2,2} & \cdots \\ d_{3,1} - d_{2,1} & d_{2,1} + d_{3,2} - d_{2,2} - d_{3,1} & d_{2,2} + d_{3,3} - d_{2,3} - d_{3,2} & \cdots \\ \vdots & \vdots & \vdots & \\ d_{h,1} - d_{h-1,1} & d_{h-1,1} + d_{h,2} - d_{h-1,2} - d_{h,1} & d_{h-1,2} + d_{h,3} - d_{h-1,3} - d_{h,2} & \cdots \end{bmatrix},$$

i.e., the elements of A are given by, using the notation $a_{i,j} = 0$ if $i < 1$ or $j < 1$,

$$a_{i,j} = h^2(d_{i-1,j+-1} + d_{i,j} - d_{i-1,j} - d_{i,j-1}) \tag{A.20}$$

In the next step, we show that all off-diagonal entries of A are negative.

Lemma 21 *If $i \neq j$, then $a_{i,j} < 0$.*

Proof For the first column, we can directly use

$$a_{i,1} = h^2(d_{i,1} - d_{i-1,1}) < 0,$$

by Lemma 20.

For $j = 2, \ldots, h-1; i = j+1, \ldots, h$, we have, by the recursive relations on the $d_{k,l}$,

$$\begin{aligned} h^{-2}a_{i,j} &= d_{i,j} + d_{i-1,j-1} - d_{i,j-1} - d_{i-1,j} \\ &= \left(1 - \frac{b}{c_{j-1}}\right) d_{i,j} + \left(\frac{b}{c_{j-1}} - 1\right) d_{i-1,j} \\ &= \left(1 - \frac{b}{c_{j-1}}\right) (d_{i,j} - d_{i-1,j}), \end{aligned}$$

the first term of which is positive by (A.18), whereas the second term is negative by (A.19). ■

We showed in Lemma 21 that

$$a_{i,i} - \sum_{j \neq i} |a_{i,j}| = \sum_{j=1}^{h} a_{i,j}.$$

Hence, we can use the structure of the entries of A, which form a telescope sum to prove that A is strictly row- (or equivalently column-) diagonally dominant.

From (A.20), we have that

$$\sum_{j=1}^{h} a_{1,j} = -h^2 d_{1,h} > 0,$$

which shows the result for the first row. For all other rows, we have

$$\sum_{j=1}^{h} a_{i,j} = h^2(d_{h,j} - d_{h,j-1}) > 0$$

by (A.19). This concludes the proof of Lemma 14.

Conclusion

The one-dimensional problem which we have investigated here has a fair amount of structure; generalizations of the results presented to two and three dimensions are important. Future work should also consider long-range interactions, nonlinear applied forces, non-local surface forces, and more general evolutions.

The choice of evolution, an H^1-gradient flow, was somewhat arbitrary from a physical point of view. Even for a static theory, the effect of the choice of evolution requires further investigation. In particular, it would be interesting to answer the question posed in Section 4.2 regarding the existence of a smooth curve leading out of the attained equilibrium state.

Acknowledgments

The initial idea for this paper arose in a discussion with Bernd Kirchheim and Georg Dolzmann about generalizations of the work of Friesecke and Theil [FT02] to realistic interaction potentials. It was taken up again and encouraged later by Johannes Zimmer. I am thankful to them for their interest and support.

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