

Resolving Structural Avalanches in Amorphous Carbon with Arclength Continuation

Fraser Birks^{1,*}, Ibrahim Ghanem², Lars Pastewka², James Kermode¹, and Maciej Buze³

¹Warwick Centre for Predictive Modelling, School of Engineering, *University of Warwick*, Coventry CV4 7AL, United Kingdom

²Department of Microsystems Engineering, *University of Freiburg*, Georges-Köhler-Allee 103, 79110 Freiburg, Germany

³MARS: Mathematics for AI in Real-world Systems, School of Mathematical Sciences,

Lancaster University, Lancaster LA1 4YF, United Kingdom



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Plastic deformation in amorphous solids is carried by localized shear transformations that self-organize into avalanches. In amorphous carbon modeled with a machine-learned interatomic potential, we find that the energetics and organization of these avalanches can be resolved by systematically following the underlying energy landscape. With a pseudoarclength numerical continuation framework, we decompose avalanches into constituent shear transformations and determine their strain-dependent energetics. Our analysis shows that, prior to onset, avalanches have a latent structure that consists of well-separated local minima. We further demonstrate that arclength continuation yields an event driven framework for following avalanche dynamics, eliminating time-step effects on statistical avalanche properties such as distributions of stress drops.

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During plastic deformation, materials undergo irreversible changes in their structure. In crystalline solids, the mechanism underlying this irreversibility is well-established: it is the glide of dislocations, line defects whose motion results in the net sliding of planes of atoms [1]. In contrast, glassy materials, which lack a periodic crystalline lattice, deform plastically through the localized yielding of small regions within the amorphous structure [2,3]. These “soft” regions, referred to as shear transformation zones (STZs), typically consist of a few tens of atoms that undergo highly nonaffine rearrangements [4].

Extensive research has been devoted to understanding the fundamental nature of STZs and determining whether there are structural indicators that can reliably predict their emergence [5]. A major challenge in this endeavor lies in the fact that STZs are not isolated entities, they interact through long-range elastic fields [6]. As a result, the activation of a single STZ can trigger the yielding of nearby regions, potentially leading to a cascade of correlated events, or structural avalanches [7]. Avalanches are most pronounced at low temperature and are often studied in athermal and quasistatic (AQS) simulations [8]. The phenomenology of systems at finite temperature and finite rate is similar, with

temperature and rate cutting off the observable avalanche sizes at small and large scales, respectively [9–12].

An AQS simulation uses sequences of finite-strain increments together with searches for the next local minimum to trace out the most likely low-temperature path of the driven system within its potential energy landscape. Figure 1 demonstrates the AQS method for computing a stress-strain curve for the simple shear of a 4096-atom sample of amorphous carbon (a-C, density 2.7 g cm^{-3}), generated via a rapid liquid quench of carbon from 10 000 K at a rate of 1000 K/ps. For interatomic interactions, we used the realistic machine-learned atomic cluster expansion (ACE) potential from Qamar *et al.* [13,14]. The stress-strain curve is shown in Fig. 1(a). Discontinuous stress drops that can be seen on this curve correspond to the activation of plastic events. Because of the covalent nature of bonding in a-C, plastic events necessarily involve the breaking and/or formation of bonds [15]. While some stress drops are associated with a single-bond rearrangement, the majority are structural avalanches involving multiple bonds. One such example is the three-bond structural avalanche highlighted in Figs. 1(c) and 1(d).

Two properties of AQS simulations limit their usefulness in the study of avalanche events: (i) the finite step size makes it difficult to determine whether events are truly correlated, or just occurring at strain values too close to resolve, and (ii) AQS simulations give no information about the inherent energetics of an avalanche, other than the trivial fact that the first barrier is zero at the instant of onset.

One way of overcoming shortcoming (ii) is to identify two mechanically stable configurations at the same applied strain before and after instability onset, and perform a

*Contact author: fraser.birks@warwick.ac.uk

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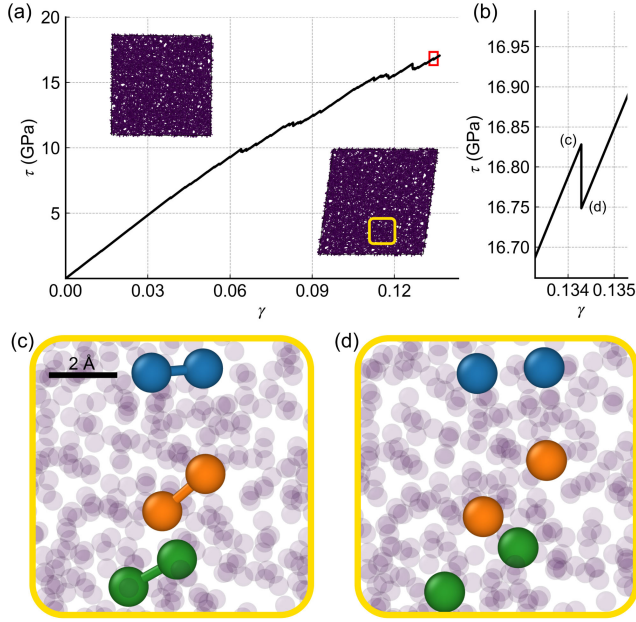


FIG. 1. Structure and plastic events in amorphous carbon. (a) The shear-stress shear-strain curve of a 4096-atom structure of amorphous carbon with a density of 2.7 gcm^{-3} . Note that γ is the applied simple shear strain. (b) An enlargement of the stress-strain curve corresponding to the position of the red box in (a). The stress drop encircled corresponds to a three-bond structural avalanche plastic event. (c),(d) The three bonds involved in the structural avalanche highlighted in (b), both before (c) and after (d) the event was triggered. The three bonds involved are colored blue, orange, and green.

nudged elastic band (NEB) [16,17] calculation to determine the minimum energy path. This approach was employed in Ref. [18] to compute the energy barriers associated with instabilities for both single shear transformations and avalanches.

We have found that while using NEB directly can work for small avalanches with fewer than three bonds involved, it is completely unsuitable for larger avalanches. There are three reasons for this: (i) many images (often > 150) are required to adequately resolve energy landscapes containing multiple intermediate minima and barriers of different sizes. (ii) Convergence frequently fails when near the avalanche onset strain. (iii) The energy pathway determined (the ordering of events) is highly sensitive to the initial guess. For further detail, see Sec. A of the Supplemental Material [19].

In this Letter, we introduce a tailored numerical arclength continuation (AC) method that overcomes the limitations of both AQS and NEB simulations. With this method, we remove step-size dependence and show that avalanches would happen in an AQS simulation even with an infinitesimally small strain step. We reveal that at strains below onset, avalanches in amorphous carbon modeled with a realistic potential decompose into latent structures

comprising chains of well-separated local minima connected by index-1 saddle points. Going further, with minimal effort, we obtain full energetic information between the intermediate basins and saddle points of the latent structure at a range of strains. Once these are identified, we validate our results by running NEB calculations between adjacent intermediate states.

AC is a method for tracking continuous solution branches of nonlinear equations as a control parameter varies [24]. In the context of amorphous plasticity, we are interested in finding sets of atomic positions $\mathbf{R} \in \mathbb{R}^{3N}$ (where N is the number of atoms) that correspond to energy minima or saddle points of a system, where all atomic forces vanish $\mathbf{F}(\mathbf{R}, \gamma) = \mathbf{0}$ simultaneously, as the applied strain γ changes. The key idea of AC is to parametrize the solution branch $\{\mathbf{R}(s), \gamma(s)\}_s$ using an arclength parameter s . In the AQS approach, the solution path $\{\mathbf{R}(\gamma), \gamma\}_\gamma$ is always parametrized by the applied strain, leading to singularities at bifurcation points, which are the critical values of the applied strain where STZs activate. In contrast, the AC approach allows a seamless traversal of the bifurcation points, meaning it is able to transition smoothly from minima to saddle (provided the interatomic potential is twice continuously differentiable in the vicinity of the bifurcation point, as is expected for any reasonable potential). The framework also admits a natural adaptive step size in s , which avoids the fixed step-size compromise inherent to AQS simulations and ensures that bifurcation events along the solution branch are not missed.

One limitation of typical AC that proves problematic in this application is the requirement for second derivative (Hessian) information. For atomistic systems, routes toward computing the Hessian are either numerical or analytical, which are both prohibitively computationally expensive for realistic interatomic potentials such as the ACE potential employed here. We therefore apply a Hessian-free pseudoarclength numerical continuation algorithm similar to that previously applied to atomistic systems by Buze and Kermode [29], with full algorithmic details presented in Sec. B of Supplemental Material [19]. AC-based approaches in atomistic modeling have also previously been explored in Refs. [30,31] to study brittle fracture and in Ref. [32] to study response of an fcc nanoslab of nickel to loading. Reference [25] also presents a related idea: the use of implicit differentiation to explore atomistic energy landscapes via a Hessian-free approximation.

We first validated this method through application to single-bond plastic events. In this system, single-bond plastic events could be broadly divided into two types: those that reversed upon strain removal (reversible events), and those that did not (irreversible events). Figure 2(a) shows the branch traversed by the continuation method for a reversible event in which a single bond forms. The solution branch has three segments. The first (lower) segment, represents an open bond, with the rightmost point

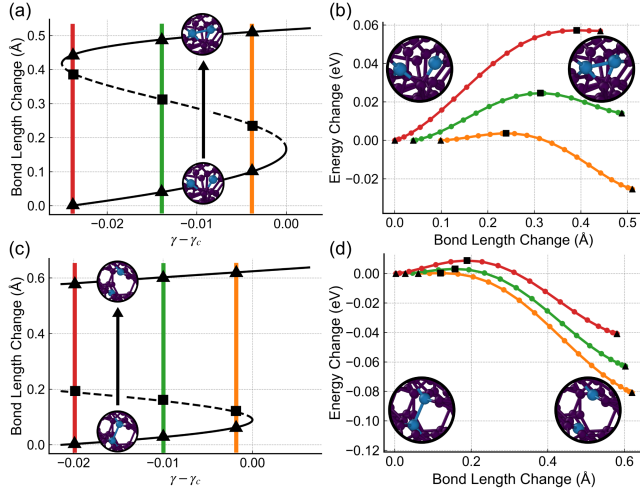


FIG. 2. The strain-dependent energy landscape of single-bond plastic events is explored using AC. (a) For a reversible event, the solution branch follows the minimum associated with the open bond (lower segment, solid black) until the critical strain γ_c , where the barrier vanishes. AC then passes through the bifurcation to the central segment, corresponding to the index-1 saddle traced as strain decreases (dashed black), before reaching the upper segment associated with the formed bond (solid black). (b) Nudged elastic band (NEB) energy profiles sampled across this landscape, with color-coded strains indicated in (a), show excellent agreement between NEB and continuation saddle energies (triangles and squares denote minima and saddles). (c),(d) The same analysis for an irreversible event shows no continuous branch from the central to the upper segment, consistent with the strongly asymmetric barrier revealed by the NEB profiles.

corresponding to the strain at which the bond would naturally form in a quasistatic simulation. After the first bifurcation point, the central segment (dashed line), where strain values retreat, represents the set of saddle points that lie between the two stable segments. Finally, after the second bifurcation point, the system reenters a minimum, with increasing strain corresponding to the further closing of the two (now bonded) atoms. Three NEB calculations across this bifurcation diagram are shown in Fig. 2(b). The strain value of each NEB calculation corresponds to the vertical line of matching color across Fig. 2(a). The energies from the continuation branch minima are marked as triangles, while the saddle energies predicted by the continuation are marked as squares.

Figures 2(c) and 2(d) demonstrate how this technique can be applied to an irreversible event. In this case, it can be seen that there is not a single continuous branch connecting stable segments. The initial procedure is the same, but rather than traversing the full branch with continuation directly, a relaxation is carried out from the saddle into the adjacent minima, effectively “jumping” the gap. By inspecting the energy landscape in Fig. 2(d) it is clear why such a gap exists: the energy barrier associated

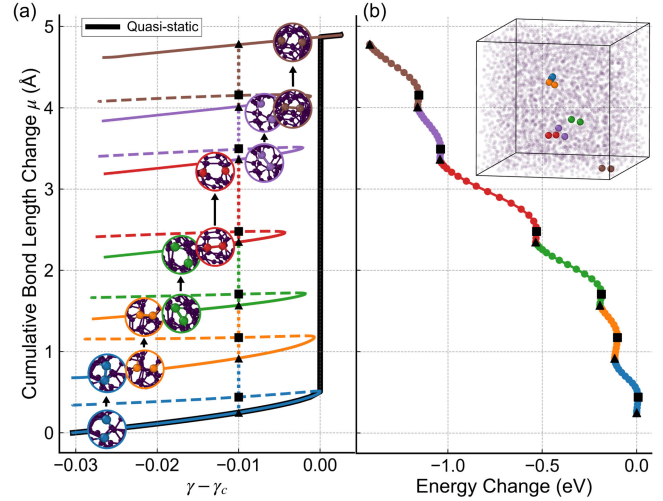


FIG. 3. The strain-dependent energy landscape of a six-bond avalanche. (a) A set of continuation branches reveals the latent structure of the avalanche. The AQS trajectory (thick black line) triggers the full avalanche at the critical strain γ_c . In contrast, AC can traverse the bifurcation at γ_c onto the index-1 saddle associated with the first bond-breaking event (dashed blue). Relaxation from this saddle at lower strain leads to an intermediate basin in which a single bond has broken (orange), and repeating this procedure (green, red, purple, and brown) resolves the avalanche into successive events. All intermediate basins disappear below γ_c , implying that even an infinitesimal-step AQS protocol would still trigger the full avalanche. (b) An NEB energy landscape at $\gamma_{xy} - \gamma_c = -0.01$, assembled from sequential NEBs between adjacent intermediate basins, with continuation minima and saddles marked by triangles and squares. The NEB and continuation saddle energies agree closely. Insets in (a) and (b) indicate the ordering of events and the full avalanche.

with the event is greatly asymmetrical, and remains similarly asymmetrical for a range of strains. In both the reversible and irreversible cases, the agreement between the NEB and continuation saddle energies is excellent.

We now turn to the complex case of traversing a multievent avalanche with AC. For visualization, we define a reaction coordinate, the cumulative active bond-length change μ , defined as $\sqrt{\sum_{ij} (r_{ij} - r_{ij}^0)^2}$, where r and r^0 refer to bond lengths in the deformed and a reference structure, respectively, and the sum runs over the “active” bonds between pairs of atoms i, j (all bonds involved in the avalanche event). Avalanche exploration proceeds through a controlled sequence of continuation and relaxation steps. As in the irreversible single-bond case, we first run continuation through the initial bifurcation point to the first saddle. Biased relaxations are performed from the saddle into the adjacent basins. Near the avalanche onset strain, the system undergoes the full cascade, but at lower strains the system lands in intermediate basins corresponding to triggering only a subset of events. For the six-bond avalanche explored in Fig. 3(a), relaxing from the first

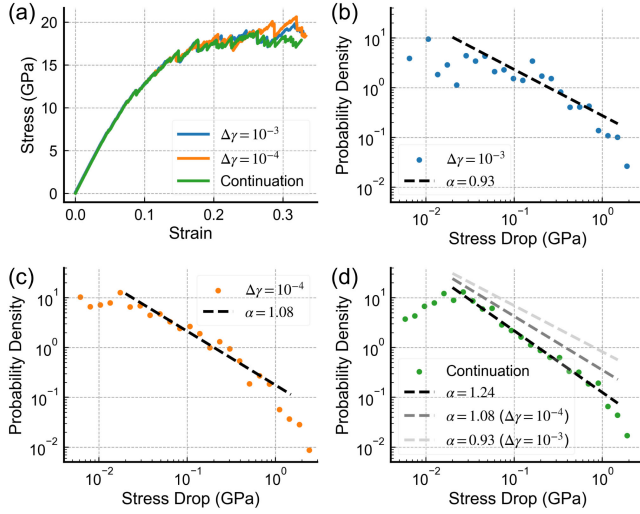


FIG. 4. Comparison between AQS and continuation simulations. (a) Overlaid stress-strain curves from AQS simulations with step sizes $\Delta\gamma = 10^{-3}$ (blue) and 10^{-4} (orange), together with continuation results (green). The curves diverge upon entering the plastic flow regime ($\gamma \gtrsim 0.17$). (b)–(d) Log-log plots of the binned probability density of stress drops for $\gamma > 0.17$ over five repeats. AQS simulation results are shown for $\Delta\gamma = 10^{-3}$ in (b) and $\Delta\gamma = 10^{-4}$ in (c); in both cases, finite step size leads to an underestimation of the exponent α of the fitted power law $p(\Delta\sigma) \sim (\Delta\sigma)^{-\alpha}$ (dashed black). In contrast, the continuation algorithm in (d) eliminates step-size dependence, yielding a steeper and more clearly defined power-law scaling.

saddle (blue dashed line) to the adjacent minima (lower orange solid line) corresponds to the triggering of only a single event. By iterating this procedure—starting from each newly discovered basin and using continuation to traverse the next saddle—we can reconstruct the avalanche as a chain of discrete transitions. In Fig. 3(a), the six-event avalanche has been dissected into six unique single-bond events colored blue, orange, green, red, purple, and brown. A full energy profile across these events formed from individual NEBs between each adjacent intermediate basin at a strain 0.01 below the onset strain γ_c is shown in Fig. 3(b). For all transitions, the continuation barrier energies agree perfectly with those predicted by each NEB calculation.

In general, we observe that avalanches cannot always be split perfectly into sequences of single-bond events; it is common for single-bond events to be so correlated that they do not disentangle even at lower strains. The range of avalanche sizes examined, together with a discussion of their degree of separability and algorithmic limitations, is provided in Sec. C of Supplemental Material [19].

Our observations highlight three interesting features of avalanches in amorphous carbon: (i) avalanches are formed from distinct sequences of low-dimensional events, (ii) these events are highly separable at strains below avalanche onset, and (iii) the sequence displays a robust internal latent structure in which the constituent events are

connected by a unique chain of local minima and index-1 saddle points. Crucially, this structure only appears below the avalanche onset strain, meaning even an infinitesimal quasistatic strain step taken at the critical strain of the first event would trigger the entire avalanche.

Going further, Fig. 4 demonstrates that continuation can not only resolve individual avalanche structures, but also yields a framework for event-driven simulation of avalanche dynamics. Panel (a) compares stress-strain curves obtained from AQS simulations with two different strain increments to the continuation result. While all curves coincide in the elastic regime, they begin to diverge upon entering steady plastic flow ($\gamma \gtrsim 0.17$), reflecting the accumulation of step-size-dependent errors in AQS simulations. Panels (b) and (c) show the corresponding stress-drop distributions measured from a number of AQS trajectories in the plastic flow regime at $\Delta\gamma = 10^{-3}$ and 10^{-4} , respectively. In both cases, the finite strain increment causes multiple nearby instabilities to be triggered within a single step, merging distinct plastic events and suppressing small stress drops. This manifests as a systematic flattening of the distribution and an apparent reduction of the exponent α of the fitted power law $p(\Delta\sigma) \sim (\Delta\sigma)^{-\alpha}$, which persists even as the step size is reduced. By contrast, panel (d) shows the distribution obtained from AC, where individual bifurcations are resolved directly. The resulting stress-drop statistics are independent of strain step size and exhibit a steeper, more clearly defined power-law scaling, indicating that continuation provides direct access to the intrinsic avalanche statistics underlying plastic flow. The step-size-independent nature of the AC method has an additional effect: it allows stress-strain curves to be reproducible with respect to small perturbations in the initial strain. This is demonstrated in Supplemental Material Sec. D [19], together with an analysis of how the computational cost of AC scales with system size and how it compares with the cost of AQS simulations.

The ability to traverse complex regions of the energy landscape for a system modeled with a high-fidelity machine-learned potential suggests that this framework is well suited to interrogate the microscopic physics of plasticity in realistic amorphous systems. In particular, as the energies of minima and saddle segments are directly attainable from continuation, this method opens the way to directly measuring how energy barriers in the system are altered by nearby plastic events; information that could be used to build accurate coarse-grained elastoplastic models or derive statistical relationships. Applying AC methods to avalanches in other glassy systems is a natural avenue for future work. Earlier studies—both in simple Lennard-Jones glasses [33–36] and in metallic glasses using embedded-atom potentials [37]—could have benefited from this approach.

Beyond these directions, the approach also has clear potential for studying more complex phenomena in

amorphous carbon, including fracture processes and the emergence of shear bands, where detailed knowledge of the underlying energy landscape could prove especially informative. It would also be valuable to relate the ordering of events identified within an avalanche's latent structure to that obtained from established avalanche discretization methods, such as overdamped dynamics [38,39]. Our preliminary analysis (see Supplemental Material, Sec. E [19]) indicates that although the two orderings are correlated, the dynamical causal chain does not always coincide exactly with the event ordering inferred from the latent structure.

In summary, we have introduced an arclength continuation-based method and applied it to investigate plastic events in amorphous carbon modeled with a machine-learned ACE potential. Unlike traditional approaches combining AQS and NEB simulations, AC is guaranteed to find bifurcation points and can directly traverse saddle points, allowing the extraction of energy barriers for each plastic event. For this realistic system, we showed that at strains below onset, avalanches can be decomposed into latent structures comprising chains of well-separated local minima connected by index-1 saddle points, the energetics of which were validated separately using NEB calculations between intermediate basins. Going further, we show that due to the elimination of step-size dependence, the adaptive AC method is particularly well suited to investigating the stress-strain response and statistics of disordered systems with plastic events that are separated by very small strain intervals. In future, we believe that AC will be a crucial tool in the investigation of avalanches in atomistic systems, and that elucidating avalanche latent structures will allow for a clearer mapping between individual rearrangements, their mutual interactions, and the collective mechanical behavior that emerges at larger scales.

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Data availability—The data that support the findings of this article are openly available [22,40].

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