Softness: a structural approach to glassy relaxation

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When a liquid freezes, a change in the local atomic structure marks the transition to the crystal. When a liquid is cooled to form a glass, however, no noticeable structural change marks the glass transition. Indeed, characteristic features of glassy dynamics that appear below an onset temperature, T_0, are captured qualitatively by mean field theory, which assumes uniform local structure at all temperatures. Even studies of more realistic systems have found only weak correlations between structure and dynamics. This begs the question: is structure important to glassy dynamics in three dimensions? Here, we answer this question affirmatively by using machine learning methods to identify a new field, ``softness," which characterizes local structure and is strongly correlated with rearrangement dynamics. We find that the onset of glassy dynamics at T_0 is marked by the onset of correlations between softness (i.e. structure) and dynamics. Moreover, we use softness to construct a simple model of slow glassy relaxation that is in excellent agreement with our simulation results, showing that a theory of the evolution of softness in time would constitute a theory of glassy dynamics.