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Breaking Propensity: A destructive method seeking structures which determine particle motion. CORDELL DONOFRIO, ERIC WEEKS, Emory University — It is known that at any given time in a supercooled liquid, particles can be found that have a higher propensity to move. This is found by running simulations with repeated initial positions but with shuffled initial velocities, and observing that some particles are in positions for which they frequently have large displacements. This suggests that local structure may play an important role, and that it may be possible to distinguish ahead of time which particles have a higher propensity for motion. We investigate the magnitude of this effect by simulating the Kob-Andersen binary Lennard-Jones glass former, and measure the propensity signal over a large range of time scales. Additionally, we attempt to 'break' this signal by introducing structural changes, thereby revealing key structural features related to propensity.

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