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Hop dynamics in glasses ANTON SMESSAERT, JÖRG ROTTLER, The University of British Columbia — Although glassy materials are widely used, we still know little about the underlying physics of the glass state. One key challenge is the non-equilibrium nature, which manifests in time-dependent material properties. A link between this "aging" and structural changes is still missing. Elementary structural relaxation events, called "hops," have been identified as particles leaving the shell of their immediate neighbors. We present first results of molecular dynamics simulations with a new algorithm that enables us to track these hops throughout the system. Using a standard polymer glass model, we show a complete "map" of the hop-dynamics in the bulk. This data allows us to explore the correlations between relaxation events. Our map of hop-events is also useful in the study of dynamical heterogeneities (DH), a concept that arose from the discovery of "faster" and "slower" moving groups of particles in glasses. Current research aims at connecting their growth to the glass transition, but their observation and study has proven to be challenging. The hop-detection gives us a coarse-grained picture of the dynamics and we can identify DH as spatio-temporal accumulations of hops. This makes a direct study of DH possible and we present preliminary results based on a cluster analysis.

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