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Ultimate self-learning metabasin escape algorithm for supercooled liquids and glasses PENGHUI CAO, HAROLD S. PARK, XI LIN, Department of Mechanical Engineering, Boston University — A generic history-penalized metabasin escape algorithm is presented in this work without any predetermined parameters. The configuration space location and volume of imposed penalty functions are determined in self-learning processes as the complete 3N-dimensional potential energy surface is sampled. The computational efficiency is demonstrated using the binary Lennard-Jones liquid supercooled to the glass transition temperature, which shows an exponential enhancement over previous algorithm implementations.

Penghui Cao
Department of Mechanical Engineering, Boston University

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