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Timewarp: Transferable Acceleration of Molecular Dynamics by Learning Time-Coarsened Dynamics

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Timewarp is an enhanced sampling method which uses a normalizing flow as a proposal distribution in a Markov chain Monte Carlo method targeting the Boltzmann distribution. The flow is trained offline on Molecular Dynamics trajectories and learns to make large steps in time (up to one ns). Crucially, Timewarp is transferable between molecular systems: once trained, it generalizes to unseen small peptides (2-4 amino acids) at all-atom resolution, exploring their metastable states and providing wall-clock acceleration of sampling compared to standard Molecular Dynamics.

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