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Gideon Simpson* (grs53@drexel.edu), Philadelphia, PA 19123. *Spin-Diffusions and Diffusive Molecular Dynamics.*

Diffusive Molecular Dynamics (DMD) is a novel approach to problems in molecular dynamics that aims to reach the diffusive time scale of milliseconds and beyond. To accomplish this, DMD “averages out” the vibrational time scale of femtoseconds and evolves probability densities at atomistic sites. This requires the approximation of a probability distribution in an extended state space by a synthetic approximate distribution, which can easily be sampled. The mean occupancy at the atomic sites are then evolved according to a system of coupled ODEs, under a so-called Master Equation, but no underlying stochastic process is given in the current formulation. In this work, we propose and examine a stochastic process, coupling a diffusion to a spin model, which gives rise to similar dynamics as DMD. This primitive model also offers a way to connect DMD to a more traditional MD. (Received March 20, 2017)