[SY-A10]Symposium A-10

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[SY-A10]Accelerating stochastic simulations with path integrals

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Monte Carlo-type simulations can extend accessible timescales c.f. atomistic models by many orders of magnitude. However, their efficiency can be significantly reduced when some of the species being simulated have very low migration barriers. This can be addressed by coarse-graining the low-barrier migration into pseudo-free continuum diffusion and, and evolving the system by drawing timesteps and hop lengths from a first passage time distribution [1,2], but this neglects the effects of spatial variation in the potential landscape in which the particles move, i.e. drift. Existing extensions require every step of a random walk to be computed, or a Fokker-Planck equation to be solved numerically [3], thus increasing the computational cost.

In this work I will describe an alternative approach, beginning from the Langevin equation for a particle moving in a general smooth potential V(x). Assuming Gaussian white noise, the stochastic equation of motion can be recast as a path integral, which can be analysed using methods borrowed from quantum field theory. Closed-form solutions for the Green function / propagator P(x,t|0,0) in a general potential are possible when the noise strength (temperature) is less than the energy scale characterising the barriers the particle has to overcome (i.e. the same range of validity as the Arrhenius rate function exp(-E/kT).) Potential applications to material simulations will be discussed.

[1] Opplestrup, Tomas, et al. "First-passage Monte Carlo algorithm: diffusion without all the hops." *Physical review letters* 97.23 (2006): 230602.

[2] Muller, Mervin E. "Some continuous Monte Carlo methods for the Dirichlet problem." *The Annals of Mathematical Statistics*(1956): 569-589.

[3] Mauro, Ava J., et al. "A first-passage kinetic Monte Carlo method for reaction-drift-diffusion processes." *Journal of Computational Physics* 259 (2014): 536-567.