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Diffusion Monte Carlo as a Stochastic Optimal Control Problem

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Solving the Schrödinger equation is a central task in quantum chemistry. Diffusion Monte Carlo (DMC) is a stochastic method that utilizes the connection between this equation and those governing diffusion phenomena to obtain accurate estimates of the eigenvalues and eigenfunctions involved.
This is made possible by the well-known Feynman-Kac formula, which allows the Schrödinger equation to be expressed in terms of the expectation of the solution to a stochastic differential equation. However, efficient evaluation of the required quantities remains an open problem. In this work, we show that bypassing the sampling from an unknown distribution with a variational principle leads to a recasting of the problem as a stochastic optimal control task. In this setting, the linearity of observables permits us to employ Koopman operator methods to approximate the desired solutions in a computationally tractable manner.

Authors: Dr NÜSKE, Feliks (Max Planck Institute for Dynamics of Complex Technical Systems); GUO, Lei (Max Planck Institute for Dynamics of Complex Technical Systems); NASCIMENTO PIRES, Luís Tadeu (Max Planck Institute for Dynamics of Complex Technical Systems)

Presenter: NASCIMENTO PIRES, Luís Tadeu (Max Planck Institute for Dynamics of Complex Technical Systems)

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