Shadow Hamiltonian dynamics for non-linear self-consistent field models

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Abstract

Molecular dynamics simulations are widely used to study systems at the atomistic scale in materials science, chemistry and molecular biology. Many models are based on a purely classical description of the potential energy surface that governs the dynamics. Such models are computationally very efficient but they cannot be used to derive important physical properties such as quantum size effects, bond formation and dissociation including charge transfer, spin-polarization, thermal or optical excitations, and various response properties such as the polarizability or the electrical conductivity. These problems all require some quantum mechanical description of the underlying electronic structure that determines the potential energy surface and the interatomic forces. Unfortunately, a quantum mechanical description based on, for example, Hartree-Fock or density functional theory, requires the solution of non-linear eigenvalue equations, which increases the computational complexity by multiple orders of magnitude. By reformulating the underlying equations to allow for the design of new solvers using data structures that are better adapted to new and emerging computer architectures, we have been able to drastically reduce the computational overhead of quantum-based molecular dynamics simulations. In this talk I will focus on recent advances and ideas on the development of the underlying molecular dynamics framework.