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Forces from stochastic density functional theory under a nonorthogonal atom-centered basis sets

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We developed a stochastic density functional theory (sDFT) approach under a nonorthogonal , atom-centered basis set representation. The method is a highly parallelizable linear-scaling approach in which the reduced scaling is achieved without imposing (or relying on) a sparse structure to the Kohn-Sham density matrix, and as such may be applicable to a wide variety of systems in biology and material science. Observables in sDFT are calculated in a trace-based formalism using the stochastic trace formula and can therefore be regarded as random variables, with an expected value and fluctuation. Due to the non-linear nature of the SCF iterations, sDFT observables are also characterized by a systematic bias error, whose magnitude can be controlled by increasing sampling as well as by employing an embedded-fragments-based, variance-reducing technique. We developed and implemented a new formalism for the calculation of forces using sDFT in the nonorthogonal, atom-centered basis set, which also includes the treatment of Pulay force terms acting on the nuclei. This is a key step towards the goal of using the "noisy"forces calculated from sDFT for geometry optimization when implemented in a Langevin dynamics framework. For this approach to be useful it is key to make sure that the systematic bias errors in the forces are sufficiently small. We present a statistical analysis of the sDFT errors in the forces acting on a Tryptophan Zipper 2 peptide solvated in water and results indicate that the sDFT bias in the forces is small and independent of system size, paving the way for future Langevin dynamics structural studies of peptides in solution.

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