# The force awakens in quantum Monte Carlo

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While quantum Monte Carlo methods are routinely employed to predict accurate total energies of relatively large systems, a major limitation has been the lack of efficient schemes to obtain energy derivatives. Here, we capitalize on a simple and general formalism we have recently developed to overcome this limitation and compute interatomic forces and other derivatives in quantum Monte Carlo with the same numerical scaling as computing the energy alone in the sampling process. These developments allow us to consistently optimize the wave function and the structural parameters in quantum Monte Carlo, and explore the performance of the method in combination with different choices of Jastrow-Slater wave functions. In particular, we show that the use of a selected-configuration-interaction scheme to generate compact and balanced determinantal components for multiple states leads to the fast and accurate computation of ground- and excited-states structures as well as vertical and adiabatic excitation energies in quantum Monte Carlo.