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Algorithmic differentiation of diffusion Monte Carlo TOM POOLE, MATTHEW FOULKES, JAMES SPENCER, PETER HAYNES, Imperial College London — Algorithmic differentiation (AD) [1] is a programming technique for the efficient evaluation of the derivatives of a computed function. This approach proceeds via the application of the chain rule to the lines of source code that constitute the mathematical operation of a computer program, allowing access to the derivatives of functions that lack an algebraic representation. Another important element of the AD method is that the "reverse mode" of operation yields the derivative of a function output with respect to all inputs, simultaneously, in a small multiple of the computational cost of evaluating the underlying function in isolation. These features make this method particularly applicable to the diffusion Monte Carlo (DMC) algorithm where, despite a number of recent advances in the area, total energy derivatives have remained problematic. Here we present results illustrating accurate DMC energy derivatives with respect to both the input wave function parameters and the nuclear positions, with the former enabling DMC wave function optimization and the latter facilitating DMC molecular dynamics simulations.

[1] A. Griewank and A. Walther, Evaluating Derivatives: Principles and Techniques of Algorithmic Differentiation, 2nd ed. (SIAM, Philadelphia IL, 2008).

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