Wave Function Optimization in QMCPACK\(^1\) JEREMY MCMINIS, University of Illinois and NCSA, MIGUEL MORALES, LLNL, JEONGNIM KIM, DAVID CEPERLEY, University of Illinois and NCSA — Wave function optimization is essential for both the accuracy and efficiency of diffusion, reptation, and variational quantum Monte Carlo (QMC). In this talk we outline the wave function optimization strategy used in the QMC software package QMCPACK developed at the University of Illinois. We use an extension of the linear optimization method originally developed by Umrigar et. al.\([1]\) to optimize parameters in Slater-Jastrow, multi-determinant Slater-Jastrow, and Backflow-Jastrow trial wave functions. The efficiency and accuracy of this method is presented for bulk Silicon, Jellium, and the Nitrogen dimer.

\[\text{[1] Umrigar et al. PRL 98, 110201 (2007)}\]

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