

Abstract Submitted
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Wave Function Optimization in QMCPACK¹ JEREMY MCMINIS,
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DAVID CEPERLEY, University of Illinois and NCSA — Wave function optimiza-
tion 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.

[1] Umrigar et al. PRL 98, 110201 (2007)

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