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Quantum Monte Carlo simulations on Blue Gene/Q using QMCPACK: Performance and Applications ANOUAR BENALI, Argonne National Laboratory, LUKE SHULENBURGER, Sandia National Laboratories, NICHOLS A. ROMERO, Argonne National Laboratory, JEONGNIM KIM, Oak Ridge National Laboratory — Quantum Monte Carlo (QMC) is the most accurate many-body method for computing ground-state properties in condensed-phase systems. QMC uses a stochastic sampling method to solve the many-body Schrödinger equation. The advent of petascale supercomputing facilities and massively concurrent QMC algorithms has allowed us to study materials at unprecedented levels of accuracy. We will present the implementation and optimization of the QMCPACK [1-2] simulation package on the IBM Blue Gene/Q as well as results for a number systems including: van der Waals-dominated materials, transition metals and biological molecules.

[1] K. Esler, J. Kim, L. Shulenburger, and D. Ceperley, Computing in Science and Engineering 14, 40 (2012).
[2] J. Kim et al., Journal of Physics: Conference Series 402, 012008 (2012).

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