

Abstract Submitted
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Extending Strong Scaling of Quantum Monte Carlo to the Exascale LUKE SHULENBURGER¹, ANDREW BACZEWSKI, Sandia National Laboratories, YE LUO, NICHOLS ROMERO, Argonne National Laboratory, PAUL KENT, Oak Ridge National Laboratory — Quantum Monte Carlo is one of the most accurate and most computationally expensive methods for solving the electronic structure problem. In spite of its significant computational expense, its massively parallel nature is ideally suited to petascale computers which have enabled a wide range of applications to relatively large molecular and extended systems. Exascale capabilities have the potential to enable the application of QMC to significantly larger systems, capturing much of the complexity of real materials such as defects and impurities. However, both memory and computational demands will require significant changes to current algorithms to realize this possibility. This talk will detail both the causes of the problem and potential solutions.

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