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Quantum Monte Carlo in the era of petascale computers JEONGNIM KIM, University of Illinois at Urbana-Champaign and Oak Ridge National Laboratory, KENNETH ESLER, Stone Ridge Technology, JEREMY MCMINIS, University of Illinois at Urbana-Champaign, MIGUEL MORALES, Lawrence Livermore National Laboratory, BRYAN CLARK, Princeton University, LUKE SHULENBURGER, Sandia National Laboratories, DAVID CEPERLEY, University of Illinois at Urbana-Champaign — Continuum quantum Monte Carlo (QMC) methods are a leading contender for high accuracy calculations for the electronic structure of realistic systems, especially on massively parallel high-performance computers (HPC). The performance gain on recent HPC systems is largely driven by increasing parallelism: the number of compute cores of a SMP and the number of SMPs have been going up, as the Top500 list attests. However, the available memory as well as the communication and memory bandwidth per element has not kept pace with the increasing parallelism. This severely limits the applicability of QMC and the problem size it can handle. (OpenMP,CUDA)/MPI hybrid programming provides applications with simple but effective solutions to overcome efficiency and scalability bottlenecks on large-scale clusters based on multi/many-core SMPs. We discuss the design and implementation of hybrid methods in QMCPACK and analyze its performance on multi-petaflop platforms characterized by various memory and communication hierarchies. Also presented are QMC calculations of bulk systems, including defects in semiconductors.

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