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Condensed Matter Applications of Quantum Monte Carlo at the Petascale¹

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Applications of the Quantum Monte Carlo method have a number of advantages allowing them to be useful for high performance computation. The method scales well in particle number, can treat complex systems with weak or strong correlation including disordered systems, and large thermal and zero point effects of the nuclei. The methods are adaptable to a variety of computer architectures and have multiple parallelization strategies. Most errors are under control so that increases in computer resources allow a systematic increase in accuracy. We will discuss a number of recent applications of Quantum Monte Carlo including dense hydrogen and transition metal systems and suggest future directions.

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