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Reducing memory demands of splined orbitals in diffusion Monte Carlo calculations[1] JARON KROGEL, FERNANDO REBOREDO, Oak Ridge National Lab — Quantum Monte Carlo calculations of defect properties of transition metal oxides have become feasible in recent years due to increases in computing power. As the system size has grown, availability of on-node memory has become a limiting factor. The main growth in memory demand stems from the B-spline representation of the single particle orbitals, especially for heavier elements such as transition metals where semi-core states are present. Despite the associated memory costs, splines are computationally efficient. In this work, we explore alternatives to reduce the memory usage of splined orbitals without significantly affecting numerical fidelity or computational efficiency. For the example case of bulk MnO we have currently achieved a memory savings of 50% while only increasing the overall computational cost of the simulation by 15%.

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