

Abstract Submitted
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An accurate, compact and computationally efficient representation of orbitals for quantum Monte Carlo calculations¹ YE LUO, Argonne National Laboratory, KENNETH ESLER, Stone Ridge Technology Company, PAUL KENT, Oak Ridge National Laboratory, LUKE SHULENBURGER, Sandia National Laboratories — Quantum Monte Carlo (QMC) calculations of giant molecules, surface and defect properties of solids have been feasible recently due to drastically expanding computational resources. However, with the most computationally efficient basis set, B-splines, these calculations are severely restricted by the memory capacity of compute nodes. The B-spline coefficients are shared on a node but not distributed among nodes, to ensure fast evaluation. A hybrid representation [1] which incorporates atomic orbitals near the ions and B-spline ones in the interstitial regions offers a more accurate and less memory demanding description of the orbitals because they are naturally more atomic like near ions and much smoother in between, thus allowing coarser B-spline grids. We will demonstrate the advantage of hybrid representation over pure B-spline and Gaussian basis sets and also show significant speed-up like computing the non-local pseudopotentials with our new scheme. Moreover, we discuss a new algorithm for atomic orbital initialization which used to require an extra workflow step taking a few days. With this work, the highly efficient hybrid representation paves the way to simulate large size even in-homogeneous systems using QMC. [1] K.P. Esler et al., Comput. Sci. Eng. 14, 40 (2012).

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