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Faster QMC with Lagrange and splines WILLIAM PARKER[1], JOHN WILKINS, Ohio State University, RICHARD HENNIG[2], CYRUS UMRIGAR[3], Cornell University — Computing the wave function can be the most time-intensive part of a quantum Monte Carlo calculation. Orbitals represented by extended basis functions scale in evaluation time as $O(N^3)$ while localized basis functions scale as $O(N^2)$. Two methods of localizing the orbital representation are: piecewise-polynomial (pp) interpolation and transformation to a localized basis. The Lagrange form of the pp-interpolant is simple but has discontinuous derivatives at sampling points. The pp-spline is continuous in certain low derivatives. The B-spline shares the pp-spline's derivative continuity but is a transformation not an interpolant. These methods have $O(N^2)$ scaling at all N tested (up to $N = 864$). While increasing the number of sampling points of the original orbital, the total QMC energy converges to the value calculated using plane waves at similar sampling point numbers for Lagrange, pp-splines and B-splines. At fixed sampling density, the three are of comparable speed. pp-splines use 8 memory words per sampling point, Lagrange use 5 and B-splines use 1. Due to smaller memory usage, B-splines are the best choice.

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