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A new algorithm for efficiently evaluating Jastrow factors in quantum Monte Carlo

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Jastrow factor is one of the keys to efficient real-space quantum Monte Carlo (QMC) simulations. It explicitly introduces electron correlation on top of mean-field orbitals to approach the exact many-body wavefunction and thus it helps reducing the variance and auto-correlation time of the statistics in QMC. The simulation efficiency is significantly improved with fewer needed samples and shorter decorrelation interval. In addition, a trial wavefunction closer to the exact ground state one has smaller locality error introduced by using pseudopotentials in diffusion Monte Carlo. For the above reasons, simulation nowadays include ion-electron, electron-electron and ion-electron-electron Jastrow factors and they consume significant amount of computational time. In this work, we introduce a new algorithm to fast update the value, gradient and Lapacian of Jastrow factors needed for computing wavefunction ratios, quantum forces and kinetic energy during single electron moves. The algorithmic complexity remains $O(N^2)$ but the memory complexity is only $\Theta(N)$ where N is the number of electrons. The highly vectorizable computation and the memory saving characteristic make it extremely efficient on modern processors with wide SIMD units and limited sized cache/high-performance memory. We achieve over 2X speed-up with the new algorithm on both electron-electron and ion-electron-electron Jastrow factors in QMCPACK and reduce the overall memory footprint by more than a half on representative simulations.