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need to employ atomic pseudo potentials. Nevertheless, Gaussian-type functions have also some disadvantages. The force calculation is more complicated, the Hartree term usually

$$v_{\mathrm{loc}}^{\mathrm{PP}}(\quad) = -\frac{Z_{\mathrm{ion}}}{}$$

er

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The computational cost of the OT method is normally dominated by the computation of the $O(\blacksquare N)$ terms and , but is in principle $O(\blacksquare N^2)$

QUICKSTEP

better than the TD scheme. The small systems with 32 and 64 H_2O scale up to 32 CPUs and the largest system with 256 $_2O$ scales even up to
However, the absolute CPU times per MD step for the TD and the PD scheme are very close, even if the PD scheme requires n the TD scheme. The PD scheme shows only for 256 H_2

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Benchmarks