Parallel in time simulations using high level quantum chemistry methods and complex empirical potentials\textsuperscript{1} ERIC BYLASKA, Pacific Northwest Natl Lab, JONATHAN WEARE, University Chicago, JOHN WEARE, UCSD — Algorithms that support parallel decomposition in the time dimension are presented and applied to conventional molecular dynamics (MD) models and \textit{ab initio} molecular dynamics (AIMD) models of realistic complexity. The algorithms support convenient parallel implementation to achieve significant improvement in the simulation of high level (e.g. MP2) and excited state dynamics. The algorithms support parallel decomposition in the time dimension are presented and applied to conventional molecular dynamics (MD) models and \textit{ab initio} molecular dynamics (AIMD) models of realistic complexity. The algorithms support convenient parallel implementation to achieve significant improvement in the simulation of high level (e.g. MP2) and excited state dynamics. The algorithms support convenient parallel implementation to achieve significant improvement in the simulation of high level (e.g. MP2) and excited state dynamics.

The fixed point problem is unconditionally convergent and is solved iteratively using a variety of optimization techniques, including quasi-Newton and preconditioned quasi-Newton methods. The algorithm is parallelized by assigning a processor to each time-step entry in the columns of $F(X)$. Less accurate but more efficient dynamical models based on simplified interactions or coarsening time-steps provide preconditioners for the root finding problem and lead to an algorithm similar to the parareal algorithm.

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