Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Parallel in time simulations using high level quantum chemistry methods and complex empirical potentials[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 *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. Given a forward time integrator propagating the system from time t_i (trajectory position and velocity $\mathbf{x_i} = (\mathbf{r_i}, \mathbf{v_i})$) to t_{i+1} as $\mathbf{x_{i+1}} = \mathbf{f_i}(\mathbf{x_i})$, the dynamics problem is transformed into a root finding problem, $\mathbf{F} = [\mathbf{x_i} - \mathbf{f}(\mathbf{x_{(i-1)}})]_\mathbf{i} = \mathbf{0}$, for the trajectory variables. 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 $\mathbf{F}(\mathbf{X})$. 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.

[1]supported by ASCR Petascale Tools program and the BES Geosciences program of the U.S. Department of Energy,

Eric Bylaska
Pacific Northwest Natl Lab

Date submitted: 15 Nov 2013 Electronic form version 1.4