FAST ALGORITHMS FOR *AB INITIO* MOLECULAR DYNAMICS

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We have developed a variety of novel algorithms for efficient propagation of classical molecular dynamics using electronic structure potentials, both at the self-consistent field level and beyond. One method, an extended Lagrangian algorithm, is inspired by Car-Parrninello molecular dynamics but employs atom-centered Gaussian orbitals rather than plane wave basis functions. This extends exisiting linear-scaling density functional theory algorithms, developed in our group, into the realm of *ab initio* molecular dynamics. An alternative set of techniques that accelerate molecular dynamics simulations employing post-Hartree-Fock electronic structure theory has also been developed, and can greatly expedite the fitting of accurate potential energy surfaces. We will survey these developments, as implemented in the Q-CHEM electronic structure program.