

# SCALABLE MOLECULAR DYNAMICS METHODS FOR REACTIVE FORCE FIELDS

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In recent years, growing interest in accurate large-scale atomistic simulation of complex material behavior has driven the development of reactive force fields (FFs) that include key physics not present in traditional interaction potentials (e.g. effects of charge transfer, local coordination and chemical bonding). These force fields tend to be computationally expensive and difficult to implement in existing parallel molecular dynamics codes. As a result, simulations with reactive force fields are often limited to short timescales and small systems sizes. We describe the development of a new massively parallel MD code for simulating large-scale atomistic systems using reactive FFs. The code is intended to be flexible enough to allow a wide range of reactive force field features to be implemented with little effort, while still providing reasonable serial efficiency and good parallel scaling. Of particular importance are three-body non-bonded interactions, bond order potentials, and charge equilibration (QE), none of which are treated by established parallel MD codes. The first two items are short range interactions used to build in coordination and chemical bonding effects. Efficient implementation will require a clean separation between force calculations and the rest of the MD code. Parallelization will present some performance issues, but there are no fundamental obstacles to parallel scaling. In contrast, QE describes the long range effect of electric field on the distribution of charge over the atoms in the system. This is essential for treatment of systems such as Si/SiO<sub>2</sub> interfaces, where atom charges vary with the local environment. Two distinct methods can be used to calculate the atom charges: explicit energy minimization (EEM) and the Car-Parrinello method (CP). Both methods have strengths and weaknesses, and efficient parallel implementation is non-trivial. EEM requires either solving a linear system of size  $N$  or performing a nonlinear optimization in  $N$  variables with one constraint. CP treats the atom charges as additional dynamic variables, which makes it faster than EEM, but less accurate. We intend to implement both of these methods. The new code will adopt established scalable parallel algorithms for long-range electrostatic forces and non-bond interactions. Additional features will be added as customer requirements dictate. The ability to treat charge transfer, local coordination, and chemical bonding that this code will provide will be of benefit to modeling of semiconductors, ceramics, metals, chalcogenides, energetic materials and water at surfaces. Materials modeling applications of particular interest include phase change behavior of Ge/Sb/Te alloys and hydrogen chemistry at the Si/SiO<sub>2</sub> interface.