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ACCELERATED MOLECULAR DYNAMICS METHODS FOR MODELING CHEMICALLY REACTIVE SYSTEMS

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ABSTRACT Accelerated molecular dynamics (AMD) methods refers to a class of techniques which enable molecular level simulation of nanoscale phenomena for long timescales (of nanoseconds to a few microseconds), by making use of novel statistical principles and high-performance computing algorithms. Typical molecular dynamics (MD) simulation makes use of particle tracking algorithms and integrates stiff Newton's laws of motion using a small timestep (femtoseconds). Traditionally, MD simulations have been applied to investigate processes that take place on very short timescale (picoseconds to a nanosecond) due to this limitation. However, several thermally activated processes at nanoscale require molecular simulations to longer timescales – a regime which is impractical to achieve via MD. In physical systems that involve chemical reactions, for example, fuel combustion, pyrolysis and polymer degradation, MD simulations for long timescale phenomenon is even more prohibitive.

In this work, we discuss a recently developed computational framework which uses AMD principles in conjunction with reactive force fields to simulate chemical reacting systems for longer time. The framework is applicable to simulate combustion chemistry, biochemistry, and material degradation phenomenon at nanoscale. We discuss the developed methodology, algorithmic aspects and application of the resulting toolkit to a sample problem of polymer degradation in ablative heatshield materials.