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Increasing the power of accelerated molecular dynamics methods and plans to exploit the coming exascale[1]

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Many important materials processes take place on time scales that far exceed the roughly one microsecond accessible to molecular dynamics simulation. Typically, this long-time evolution is characterized by a succession of thermally activated infrequent events involving defects in the material. In the accelerated molecular dynamics (AMD) methodology, known characteristics of infrequent-event systems are exploited to make reactive events take place more frequently, in a dynamically correct way. For certain processes, this approach has been remarkably successful, offering a view of complex dynamical evolution on time scales of microseconds, milliseconds, and sometimes beyond. We have recently made advances in all three of the basic AMD methods (hyperdynamics, parallel replica dynamics, and temperature accelerated dynamics (TAD)), exploiting both algorithmic advances and novel parallelization approaches. I will describe these advances, present some examples of our latest results, and discuss what should be possible when exascale computing arrives in roughly five years.

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