The Improvement of Length Scaling in the Hyperdynamics Method
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National Laboratory — Many important physical phenomena, such as film growth,
bulk diffusion, radiation damage annealing, dislocation climb and catalysis, require
both long time scale and large length scale molecular dynamics, where conventional
molecular dynamics methods are not applicable due to the computational costs. The
hyperdynamics method has enabled us to perform molecular dynamics for a longer
time scale. However, this method is limited in length scale because the overall com-
putational speedups achieved by the current bias potential methodologies decrease
rapidly with the size of the system. To overcome this disadvantage, we are designing
new bias potential methodologies to maintain the overall computational speedup in
larger systems. We calculate the hyperdynamics rates and the overall speedups with
the current and new approaches and discuss the fundamental aspects of both ap-
proaches. The early results show that these new methods are promising for reaching
greater time and length scales simultaneously.