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The Improvement of Length Scaling in the Hyperdynamics Method SOO YOUNG KIM, ARTHUR VOTER, Theoretical Division, Los Alamos 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 computational 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 approaches. The early results show that these new methods are promising for reaching greater time and length scales simultaneously.

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