To overcome time-scale gap

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Time-scale gap between experiment and MD

- Experiments 1s-1h
- Molecular Dynamics -1ns

- Direct comparison is meaningless!
  - Need to establish the concept to bridge the time-scale

Accelerated MD

- Metadynamics (A. Laio,M. Parrinello, PNAS 99(2002), 12562)
- Self-guided MD (Used by P. Clancy JCP 122(2005)154509)
- Hyperdynamics (Used by P. Clancy JCP 122(2005)154509)
- Eigen-vector following BFGH scheme (T. Middleton, D. Wales, PRB 64(2001) 024205)

Metadynamics

- Fill the minima in the FES (free-energy surface) by Gaussian function-like energy (force, which does not allow the system to revisit the same (previous) configuration.

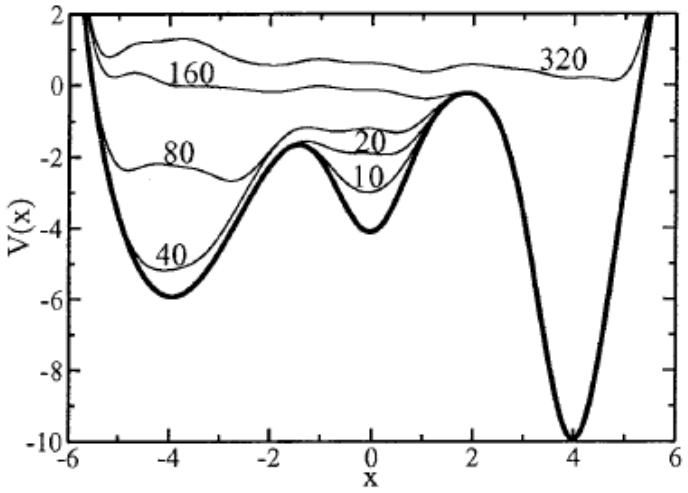

Fig. 1. Time evolution of the sum of a one-dimensional model potential $V(\sigma)$ and the accumulating Gaussian terms of Eq. **2**. The dynamic evolution (thin lines) is labeled by the number of dynamical iterations (Eq. **1**). The starting potential (thick line) has three minima and the dynamics is initiated in the second minimum.

•Can obtain Saddle-point energy (not reaction path) and local (global) minimum energies and configurations

•Through the combination with nudged-elastic band method, one can obtain the reaction path

Metadynamics

- Applications
  - Transformation of SiO2 under various pressure (Nature materials, vol. 5(2006)635)
  - Ice nucleation (JCP 123(2005)051108, 124(2006)204705)
  - New Parrinelo-Rahman method (PRL 90(2003)075503)
  - Other discussions (PRL 92(2004)170601, PRL 96(2006)090601)

Application to amorphous silicon

- Self-guided MD and hyperdynamics
  (D. Choudhary, P. Clancy JCP 122 (2005) 154509)
- EF/BFGS method
  (T. Middleton, D. Wales, PRB 64(2001) 024205) also applied to binary LJ system
  – There are two kinds of relaxation, nondiffusive and diffusive process, which make the relaxation phenomena complicated.

Difficulty in amorphous relaxation

- There might be many local minimum configurations which cannot access to (or require significant calculation time to access to) in the framework of the molecular dynamics
- There is a possibility that accelerated schemes find out such configurations.

Effectively of accelerated MD

- To look for wide variety of configuration space
- To find out unknown reaction path and lower energy state
- To connect nudge-elastic band scheme easily