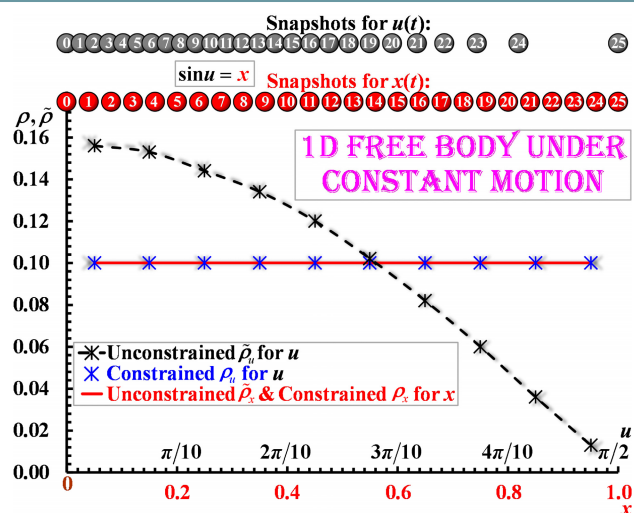


FULL PAPERS



Zero force can produce an infinitely-high energy barrier?! It sounds impossible, but it could be true based on a conventional free-energy profile generated from unconstrained probability-density $\tilde{\rho}$ simulations (see Figure). By contrast, no energy barrier is found based on any constrained

free-energy profiles. This is an excellent simplest example to pinpoint elementary differences between the nature of unconstrained and constrained results, and thus, to overturn the conventional wisdom that the unconstrained is thought to be the superior one.

Prof. K.-Y. Wong*, Dr. Y. Xu, Dr. L. Xu

1 – 22

Pitfall in Free-Energy Simulations
on Simplest Systems



Free Clip of Video Abstract:
which is available on three platforms:

(i) <https://youtu.be/K614dbSGKrk>

(ii) <https://vimeo.com/222712474>
(with an official "Download" link)

(iii) <https://bcove.video/2toHOXP>

DOI: 10.1002/slct.201601160