

A Quadratic String Adapted Barrier Exploring Method for Locating Transition States

Daewon Lee^{a,*}, Jaewook Lee^a, Young-Gui Yoon^b

^aInformatics Laboratory, POSTECH, Republic of Korea

^bDepartment of Physics, Chung-Ang University, Republic of Korea

This paper proposes a novel method for locating relevant transition states that contain crucial information on rare events of transition from the energy barriers, such as ionic diffusion in a crystalline material with vacancies and adatom migration at surfaces. Figure 1 illustrates the proposed method. Given two adjacent stable states A and B , we first locate an initial barrier state BS_0 that takes the maximum energy values along the straight line connecting A and B . Then BS_0 is driven by a force for some time period and arrives at a temporal state M_1 . We next locate a barrier state BS_1 that takes the maximum energy values along a quadratic string curve passing through A , B , M_1 . This procedure is repeated until a relevant transition state is located. Table 1 demonstrates that the proposed method successfully locates the transition states for the benchmark energy surface problems [4,5]: Muller-Brown (MB), Eckhardt (EC), Minyaev-Quapp (MQ), Gonzales-Schlegel (GS), Neria-Fischer-Karplus (NFK) [4] and -F1, F9 surface.

This work was supported by the KOSEF under the grant number R01-2005-000-10746-0.

REFERENCES

1. Nusse et al, Science 271 (1996) 1376.
2. Passerone et al, Phys. Rev. Lett. 87 (2001).
3. Henkelman et al, Progress on Theo. Chem. and Phy. (2000).
4. Quapp et al, J. of Com. Chem. 19 (1998) 9.
5. Renka et al, ACM Trans. on Math. Soft. 25 (1999) 1.

*Corresponding author (woosuhan@postech.ac.kr).

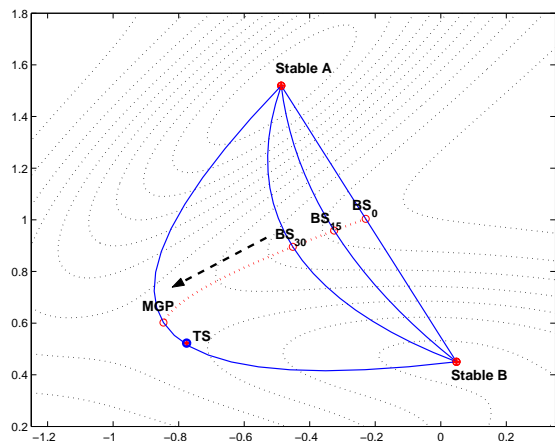


Figure 1. Contour plot of the Muller-Brown energy surface. Where BS_i are generated barrier states and TS is a transition state between two stable states, A and B , obtained by the proposed method.

Table 1
Experimental Results.

F	Energy values on ($A \rightarrow TS \rightarrow B$)
MB	(-203.8 \rightarrow -112.5 \rightarrow -114.1)
MB	(-187.5 \rightarrow -75.0 \rightarrow -114.1)
EC	(0.000 \rightarrow 2.041 \rightarrow 0.000)
MQ	(0.000 \rightarrow -1.430 \rightarrow 0.000)
NFK	(0.000 \rightarrow -0.002 \rightarrow 0.000)
-F1	(-1.220 \rightarrow -0.501 \rightarrow -0.643)
F9	(-1.986 \rightarrow -0.951 \rightarrow -1.271)