Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

An improved Activation-Relaxation Technique method for finding transition pathways[1] FREDERIC LEGOLL, Ecole Nationale des Ponts et Chaussees — The Activation-Relaxation Technique nouveau (ARTn) is an eigenvector following method for systematic search of saddle points and transition pathways on a given potential energy surface. We propose a variation of this method aiming at improving the efficiency of the local convergence close to the saddle point. The efficiency of the method is demonstrated in the case of point defects in body centered cubic iron. We also prove the convergence and robustness of a simplified version of this new algorithm. Joint work with E. Cances, M.-C. Marinica, K. Minoukadeh and F. Willaime.

[1]This work was partially supported by the Agence Nationale de la Recherche (LN3M project, Contract No. ANR-05-CIGC-0003).

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Date submitted: 10 Nov 2011 Electronic form version 1.4