An improved Activation-Relaxation Technique method for finding transition pathways\textsuperscript{1} FREDERIC LEGOLL, Ecole Nationale des Ponts et Chaussées — 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.

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