

# Demo MATLAB codes for finding transition paths and transition states

## Codes for finding saddles

`dimer_demo.m` and `dimer_demo1.m` implement the shrinking dimer method [ZD] for finding Morse index one saddles in a 2D three-well potential.

`dimer_demo.c` starts with finding MEPs (minimum energy paths) using the string method and then nails down saddles using the shrinking dimer method. `dimer_demo1.m` runs the shrinking dimer method starting from a set of uniformly distributed locations in the computational domain.

## Codes for finding MEPs (minimum energy paths)

`string_7well.m` implements the string method to find MEPs between all pairs of local minima in a 2D seven-well potential [ERV].

`NEB_demo_2well.m` implements the nudged elastic band method [JMJ] to find the MEP connecting the minima in a 2D double-well potential.

## Codes for finding MEPs for SPDEs

`AllenCahnString.m` implements the string method to find a MEP in the 2D Allen-Cahn model [AC]

## Codes for finding MAPs (minimum action paths)

`gma.m` implements the geometric minimum action method [HV] for finding a MAP connecting the asymptotically stable equilibria in the bistable Maier-Stein system [MS]

## References

- [ZD] J. Zhang, Q. Du, Shrinking dimer dynamics and its applications to saddle point search, *SIAM J. Numer. Anal.*, 50, 4, 1899–1921 (2012)
- [ERV] W. E, W. Ren, E. Vanden-Eijnden, Simplified and improved string method for computing the minimum energy paths in barrier-crossing events. *J. Chem. Phys.* 126, 164103 (2007)
- [JMJ] H. Jonsson, G. Mills, K. W. Jacobsen, Nudged elastic band method for finding minimum energy paths of transitions. In: Berne, B.J., Ciccoti, G., Coker, D.F. (eds.) *Classical and Quantum Dynamics in Condensed Phase Simulations*, p. 385. World Scientific, Singapore (1998)
- [AC] S.M. Allen, J.W. Cahn, A microscopic theory for antiphase boundary motion and its application to antiphase domain coarsening, *Acta Metall.* 27 (1979) 1085–1095
- [MS] R. Maier and D. Stein, A scaling theory of bifurcations in the symmetric weak-noise escape problem, *J. Statist. Phys.* 83, no. 3-4, 291–357 (1996)