Supplemental Information: Identifying Reaction Pathways via Asymptotic Trajectories

Yutaka Nagahata,¹ F. Borondo,^{2,3} R. M. Benito,⁴ and Rigoberto Hernandez^{1,*}

¹Department of Chemistry, Johns Hopkins University, Baltimore, MD 21218 ²Instituto de Ciencias Matemáticas (ICMAT), Cantoblanco, 28049 Madrid, Spain ³Departamento de Química, Universidad Autónoma de Madrid, Cantoblanco, 28049 Madrid, Spain ⁴Grupo de Sistemas Complejos, Escuela Técnica Superior de Ingeniería Agronómica, Alimentaria y de Biosistemas, Universidad Politécnica de Madrid, 28040 Madrid, Spain (Dated: November 17, 2019)

ANIMATED GIFS

Associated with this document are the following four animated gif files:

- Alg.gif: Step-by-step visualization of the NBC-ATI algorithm also shown in Fig. 6 in the main text.
- 2. prop.gif: Backward/forward propagation in time of the stable (blue,cyan) and unstable (red/orange) manifolds of the 1D ketene model with external force. The initial samples of manifolds are obtained from the algorithm explained in Fig. D2. The colors of the manifolds get lighter, as |t| increases. The snapshot of the figure is also shown in Fig. D.4 in the appendix.
- 3. turnstile_w_coherent.gif: Turnstile structure shown in Fig. 11 of the main text

but in blue (top) and red (bottom)

4. combine_w_energy.gif: (Top) The potential energy surface of the ketene 1D model with time-dependent external field (also shown in Fig. 1(a)), and external force (background color: negative (blue) and positive (red)), trajectories (blue and red circles) and their path (blue and red dots) with the total energy. (Middle, Bottom) The periodical motion of the stable (blue, cyan) and unstable (red, orange) manifolds, coherent sets of trajectories (red, blue areas). The snapshot of the figure is also shown in Fig. 13(a), and b. The energy of a trajectory changes only when the trajectory path through the colored area in the top figure.

^{*}r.hernandez@jhu.edu