String Method in Collective Variables (SMCV)
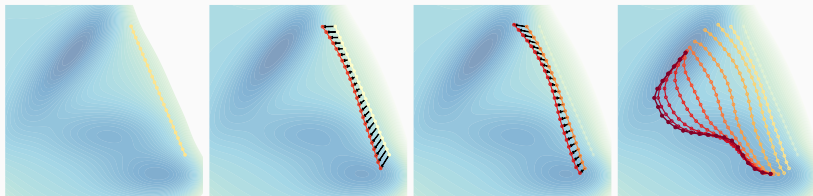
A convergent approach to find minimum free-energy (reversible) pathways in feature space represented by sequences of system **images**

Initial image positions: $\{\boldsymbol{z}\}(0) \equiv \{\boldsymbol{z}_1(0), \boldsymbol{z}_2(0), \ldots, \boldsymbol{z}_M(0)\}$

Image updates: $\{\boldsymbol{z}\}(t + \Delta t) = \{\boldsymbol{z}\}(t) - \Delta t \dfrac{\partial F}{\partial \{\boldsymbol{z}\}} + \text{reparam.}$

Mean forces on image i: $-\dfrac{\partial F}{\partial \boldsymbol{z}_i} = \langle \kappa \left[\boldsymbol{\theta}_i(\boldsymbol{x}_i) - \boldsymbol{z}_i\right] \rangle_{\boldsymbol{z}_i}$

found by restrained MD: $\langle \kappa \left[\boldsymbol{\theta}_i(\boldsymbol{x}_i) - \boldsymbol{z}_i\right] \rangle_{\boldsymbol{z}_i} = \dfrac{1}{N_s} \sum\limits_{j=1}^{N_s} \kappa \left\{ \boldsymbol{\theta}_i[\boldsymbol{x}_i(t_j^{MD})] - \boldsymbol{z}_i \right\}$

Temporary page!

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