# Aggregation free energy landscape along the committor - the optimal reaction coordinate

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Projecting multidimensional dynamics of a complex system onto reaction coordinates (RCs) is a common and usually necessary approach for describing such systems. Then, one is usually interested in describing the system's kinetics looking only at those projections. To achieve that, some stochastic model over that coordinate is usually considered so that the other degrees of freedom are modeled as noise. The simplest of such stochastic models is the diffusive model defined by the Smoluchowski equation. As there is no guarantee that usual physically motivated RCs can be employed within that simple model, the choice of the RC is a crucial step in order to achieve a proper description of the system. For systems describing transitions between two boundary states, the committor function is an optimal coordinate. That is because important kinetic properties can be computed exactly using the committor projection within the diffusive model. The committor equals the probability of reaching one boundary state before the other one given that the system is at an arbitrary configuration. While the system's description along the committor projection is appealing straightforward due to its connection with simple one-dimensional diffusion, the computation of the committor itself is much more challenging. Recently, a variational approach for constructing the committor time series were proposed and successfully applied for protein folding [1], in which the native and denatured states serves as the boundary states. Here, we applied that technique and were able to obtain the accurate committor free energy landscape for a lattice system with anisotropic interactions [2] undergoing aggregation transitions. For this system, diluted and aggregated states serve as the boundary states and, we were able to calculate kinetic properties of the transitions between those states from the constructed committor landscape. For the same system, we have also shown recently that using energy as RC led to an accurate kinetic description at high temporal scales [3]. Here, usage of the committor prevents the need of such timescale separation. This work presents a general procedure for constructing the optimal RC for aggregation systems containing many particles, and we hope that it might also be suitable for more realistic systems. **Financial support**: FAPEMIG, CAPES, CNPq.

## References

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