# 8. Summary and Conclusion

In this thesis, we have presented the framework of transition path theory (TPT) for time continuous Markov processes with continuous and discrete state space. TPT provides statistical properties of the ensemble of reactive trajectories between some start and target sets and yields properties such as the committor function, the probability distribution of the reactive trajectories, their probability current and their rate of occurrence. We have shown that knowing these objects allows one to arrive at a complete understanding of the mechanism of the reaction.

The main objects of TPT for Markov diffusion processes have been explicitly derived for the Langevin and Smoluchowski dynamics and we have illustrated them on a various number of low-dimensional examples. Despite the simplicity of these examples compared to those encountered in real applications, they already demonstrate the ability of TPT to handle complex dynamical scenarios. The main challenge in TPT for diffusion processes is the numerical computation of the committor function as a solution of a Dirichlet-Neumann boundary value problem involving the generator of the process.

Beside the derivation of TPT for Markov jump processes, we have focused on the development of efficient graph algorithms to determine reaction pathways in discrete state space. One approach via shortest-path algorithms has turned out to give only a rough picture of possible reaction channels whereas the network approach allows a hierarchical decomposition of the set of reaction pathways such that the dominant channels can be identified. We have successfully applied the latter approach to an example of conformational dynamics of a bio-molecule. In particular, we have made use of a maximum likelihood method to estimate the infinitesimal generator of a jump process from an incomplete observation. Finally, we have addressed the question of error propagation in the committor function computation for Markov chains.

The discrete TPT framework has many interesting relations to other topics in the Markov chain and network literature; we have briefly discussed the relation to electric resistor network theory and data segmentation tools such as Laplacian eigenmaps and diffusion maps. Future investigations should work out these and other relations in more detail.