Chapter 4

Concluding Remarks

This thesis deals with averaging and related asymptotic techniques for the elimination of fast DOF in (stochastic) dynamical systems. It is motivated by the article [43] which builds on the observation that the available techniques can be inappropriate if the fast degrees of freedom induce very long transition time scales due to metastability effects. These cases may appear in real-life applications, e.g., in molecular dynamics with fast torsion angle dynamics. The authors of [43] have derived indicators for the possible inadequacy of the averaging scheme for simple diffusion processes, and have constructed an extension of the averaging technique for cases where metastability in fast modes causes the longest time scales in the system. As a result they obtained the principle of Conditional Averaging that –under certain circumstances– yields an appropriate model in cases where the "usual" averaging principle fails. Moreover, the resulting numerical scheme can be handled almost as easily as the usual averaging scheme. The manuscript at hand is concerned with the Conditional Averaging scheme by considering it through a fine-grained perspective as well as reconsidering the the asymptotic procedure in a more rigorous setting that yields results beyond the scope of Conditional Averaging.

The setting where Conditional Averaging is appropriate is illustrated in Figure 4.1, where we observe a metastable decomposition that does not depend on the slow variable x. Then, we can describe the effective dynamics over ord(1) time scale by averaging out the fast dynamics in y conditioned upon remaining within one metastable set. The exchange between the two reduced models is quantified by a rate matrix that is given in terms of the second eigenvalue of the fast dynamics' generator.

The approach 'Replacing fast dynamics by coupled OU processes' in the first part of the thesis is motivated by the desire for a thorough understanding of the conditionally averaged dynamics. It builds on a direct analysis of the single system dynamics that is described by the Smoluchowski equation. The fundamental idea is to extract the transition behaviour between the

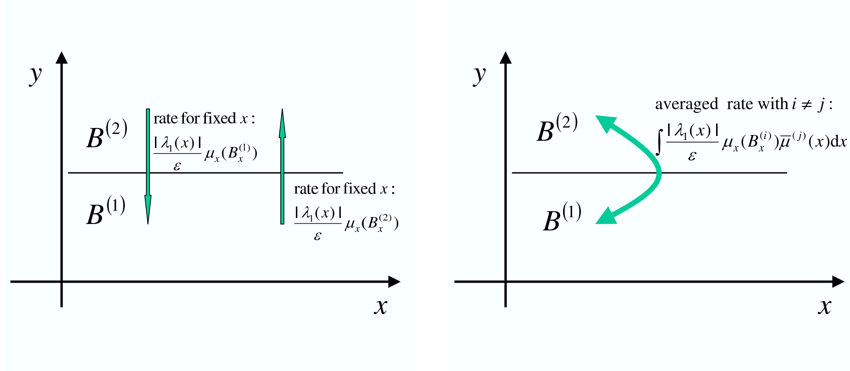

Figure 4.1: Metastable subsets $B^{(1)}$ and $B^{(2)}$ are independent of x. Left: Conditional Averaging scheme, where the transition rates between the metastable subsets depend on the slow variable x; they reproduce the transition behaviour on every fibre of the fast state space. Right: Under certain circumstances (invariant density restricted to $B^{(1)}$ and $B^{(2)}$, respectively, is entirely sampled before any transition happens), we obtain the transition rates between the subsets $B^{(1)}$ and $B^{(2)}$ as averages of the x-dependent rates that are illustrated on the left-hand side.

metastable fast dynamics "manually", which then allows the replacement of the fast dynamics within the metastable subsets by (irreducible) OU processes. We thus arrive at a system of fast-slow equations where the fast dynamics are governed by coupled OU processes, respectively, and where a transition matrix describes the transitions between the different OU processes. A reduced system is then obtained by averaging out the fast variable in each of the fast-slow equations according to the invariant measure of the corresponding OU process. The ansatz provides a deep insight into the origin of the rate matrix from the Conditional Averaging scheme. It enables us to draw conclusions about the asymptotic position of the boundary between the metastable subsets, information which has not been provided by the formal strategy of Conditional Averaging. All these results have been illustrated by appropriate numerical experiments, which nicely round off the approach.

The approach 'Multiscale asymptotics with disparate transition scales' that is pursued in the second part of the thesis is based on a formal asymptotic strategy that allows the derivation of averaged models for various kinds of scenarios that go beyond the simple Conditional Averaging scheme. As illustrated in Fig. 4.2, we allow the metastable decomposition to depend on the slow variable x which requires the time scale over which the dynamics induce metastable transitions to be more flexibly linked with the time scales of the x and y dynamics. In so doing, we distinguish between transitions induced by the y dynamics and transitions along the x direction. Over order unity time scale we then retain the averaged Fokker-Planck generators from the Conditional Averaging scheme where each is connected to one metastable

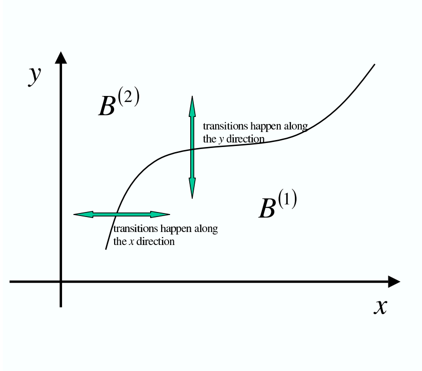

Figure 4.2: Metastable subsets $B^{(1)}$ and $B^{(2)}$ can also depend on x.

subset. The exchange between the metastable subsets now depends on the dynamical facets of the dynamics, where only one of the possible situations recovers the conditionally averaged dynamics. The extended results now include the situation where the metastable transitions happen on a longer time scale: There are two rate matrices available, where one reproduces the metastable transitions along the y dynamics (which now are independent of x) as illustrated in the right picture of Fig. 4.1, and the other describes the transitions that are induced by the effective x dynamics.

We have stopped short of demonstrating the feasibility of the above derived reduced models on the basis of appropriately chosen numerical examples. It is our belief that it can be a challenging task to decide which scenario will be appropriate for a given potential, and that the study of numerical applications would therefore go beyond the scope of this thesis. Also, we have not shown that all these cases and orderings can actually happen in practice. Therefore, the problems that aim directly for the numerical feasibility, such as the construction of examples tailored to the different cases, should by accomplished elsewhere.