16 Conclusion

It is useful to construct slow invariant manifolds. Effective model reduction becomes unfeasible without them for complex kinetic systems.

Why should we attempt to reduce the description in the times of supercomputers?

- First, in order to gain insight. In the process of reducing the description we is often able to extract the essential, and the mechanisms of the processes under study become more transparent.
- Second, once we obtain the detailed description of the system, then we can try to solve the initial-value problem for this system. But what should one do in the case where the system represents just a small part of the huge number of interacting systems? For example, a complex chemical reaction system may represent just a point in a three-dimensional flow.
- Third, without reducing the kinetic model, it is impossible to construct this model. This statement seems paradoxical only at the first glance: How can it come, the model is first simplified, and is constructed only after the simplification is done? However, in practice, the statement of the problem typical for a mathematician (Let the system of differential equations be *given*, then ...) is rather rarely applicable for detailed kinetics. On the contrary, the thermodynamic data (energies, enthalpies, entropies, chemical potentials etc) for sufficiently rarefied systems are quite reliable. Final identification of the model is always done on the basis of comparison with the experiment and with the help of fitting. For this purpose, it is extremely important to reduce the dimension of the system, and to reduce the number of tunable parameters.
- And, finally, for every supercomputer there exist problems that are too complicated. Model reduction makes these problems less complicated and sometimes gives us the possibility to solve them.

It is useful to apply thermodynamics and the quasiequilibrium concept while seeking slow invariant manifolds. Although open systems are important for many applications, it is useful to begin their study and model reduction with the analysis of closed (sub)systems. The thermodynamics equips then these systems with the Lyapunov functions (entropy, free energy, free enthalpy, depending on the context). These Lyapunov functions are usually known much better than the right hand sides of kinetic equations

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(in particular, this is the case in reaction kinetics). Using a Lyapunov function, one constructs the initial approximation to the slow manifold, that is, the quasiequilibrium manifold, and also one constructs the thermodynamic projector.

The thermodynamic projector is the unique operator which transforms the arbitrary vector field equipped with the given Lyapunov function into a vector field with the same Lyapunov function (and also this happens on any manifold which is not tangent to the level of the Lyapunov function).

The quasi-chemical approximation is an extremely rich toolbox for assembling equations. It enables one to construct and study wide classes of evolution equations equipped with prescribed Lyapunov functions and Onsager reciprocity relations.

The **method of natural projector** is an attractive method of model reduction for dissipative systems, and at the same time it gives a clue to the problem of irreversibility. The formula for *entropy production*,

$$\sigma \sim \frac{\text{defect of invariance}}{\text{curvature}}$$

clarifies the geometrical sense of the dissipation. Here, "defect of invariance" is the defect of invariance of the quasiequilibrium manifold, and "curvature" is the curvature of the **film of nonequilibrium states** in the direction of the defect of invariance of the quasiequilibrium manifold

Slow invariant manifolds of thermodynamically closed systems are useful for constructing slow invariant manifolds of the corresponding open systems. The necessary technique is developed.

The ***k*-contractions** and the **quasi-biological representation** allow to find finite-dimensional asymptotics for some of infinite-dimensional systems.

The **postprocessing** of the invariant manifold construction is important both for the estimation of the accuracy and for the accuracy improvement.

The main result of this book can be formulated as follows: **It is possible indeed to construct invariant manifolds.** The problem of constructing invariant manifolds can be formulated as the invariance equation, subject to additional conditions of slowness (stability). The Newton method with incomplete linearization, relaxation methods, the method of natural projector, and the method of invariant grids enables educated approximations to the slow invariant manifolds. These methods were tested on a recently discovered class of **exactly solvable reduction problems**.

It becomes more and more evident at the present time that the constructive methods of invariant manifold are useful for a wide range of subjects, spanning from applied hydrodynamics to physical and chemical kinetics.