1 Introduction

1.1 Ideas and References

In this book, we present a collection of constructive methods to study slow (stable) positively invariant manifolds of dynamic systems. The main objects of our study are dissipative dynamic systems (finite or infinite) which arise in various problems of kinetics. Some of the results and methods presented herein may have a more general applicability, and can be useful not only for dissipative systems but also, for example, for conservative systems.

Nonequilibrium statistical physics is a collection of ideas and methods for the extraction of slow invariant manifolds. Reduction of description for dissipative systems assumes (explicitly or implicitly) the following picture: There exists a manifold of slow motions in the phase space of the system. From the initial conditions the system goes quickly in a small neighborhood of the manifold, and after that moves slowly along this manifold (see, for example, [1]). The manifold of slow motion (slow manifold, for short) must be positively invariant: if a motion starts on the manifold at t_0, then it stays on the manifold at $t > t_0$. The frequently used wording "invariant manifold" is not really precise: for dissipative systems, the possibility of extending the solutions (in a meaningful way) backwards in time is limited. So, in nonequilibrium statistical physics we study *positively invariant* (or inward invariant) slow manifolds. The necessary invariance condition can be written explicitly as the differential equation for the manifold immersed into the phase space. This picture is directly applicable to *dissipative* systems.

Time separation for *conservative* systems and the way from the reversible mechanics (for example, from the Liouville equation) to dissipative systems (for example, to the Boltzmann equation) requires some additional ideas and steps. For any conservative system, a restriction of its dynamics onto any invariant manifold is conservative again. We should represent a dynamics of a large conservative system as a result of dynamics in its small subsystems, and it is necessary to take into account that a *macroscopically* small interval of time can be considered as an infinitely large interval for a small subsystem, i.e. microscopically. It allows us to represent the relaxation of such large systems as an ensemble of *indivisible events* (for example, collisions). The Bogolyubov–Born–Green–Kirkwood–Yvon (BBGKY) hierarchy

Alexander N. Gorban and Iliya V. Karlin: *Invariant Manifolds for Physical and Chemical Kinetics*, Lect. Notes Phys. **660**, 1–19 (2005)
www.springerlink.com

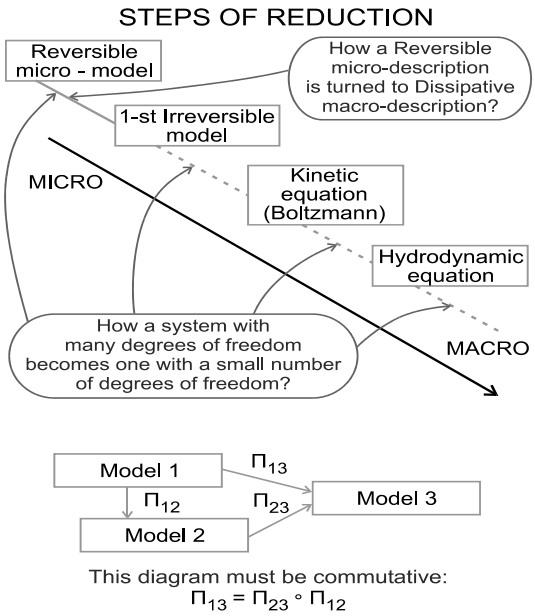

Fig. 1.1. The stairs of reduction, step by step

and Bogolyubov's method of derivation of the Boltzmann equation give us the unexcelled realization of this approach [2].

The "stairs of reduction" (Fig. 1.1) lead from the reversible microdynamics to irreversible macrokinetics. The most mysterious is the first step: the emergence of irreversibility. We discuss this problem in Chap. 12, but the main focus of our attention in the book is the model reduction for dissipative systems.

For dissipative systems, we always keep in mind the following picture (Fig. 1.2). The vector field $J(x)$ generates the motion on the phase space U: $\mathrm{d}x/\mathrm{d}t = J(x)$. An ansatz manifold Ω is given, it is the current approximation to the invariant manifold. This manifold Ω is described as the image of the map $F : W \to U$. The choice of the space of macroscopic variables W is the important step of the model reduction: all corrections of the current ansatz manifold are described as images of various F for given W.

The projected vector field $PJ(x)$ belongs to the tangent space T_x, and the equation $\mathrm{d}x/\mathrm{d}t = PJ(x)$ describes the motion along the ansatz manifold Ω (if the initial state belongs to Ω). The induced dynamics on the space W is generated by the vector field

$$\frac{\mathrm{d}y}{\mathrm{d}t} = (D_y F)^{-1} PJ(F(y)) \; .$$

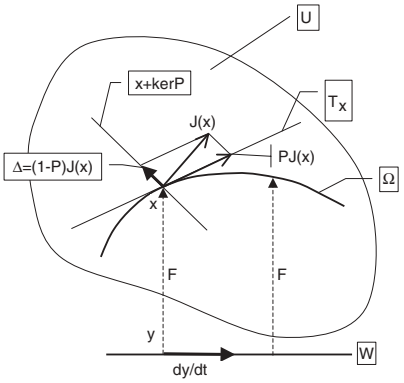

Fig. 1.2. The main geometrical structures of model reduction: U is the phase space, $J(x)$ is the vector field of the system under consideration: $\mathrm{d}x/\mathrm{d}t = J(x)$, Ω is an ansatz manifold, W is the space of macroscopic variables (coordinates on the manifold), the map $F : W \to U$ maps any point $y \in W$ into the corresponding point $x = F(y)$ on the manifold Ω, T_x is the tangent space to the manifold Ω at the point x, $PJ(x)$ is the projection of the vector $J(x)$ onto tangent space T_x, the vector field $\mathrm{d}y/\mathrm{d}t$ describes the induced dynamics on the space of parameters, $\Delta = (1 - P)J(x)$ is the defect of invariance, the affine subspace $x + \ker P$ is the plain of fast motions, and $\Delta \in \ker P$

Here the inverse linear operator $(D_y F)^{-1}$ is defined on the tangent space $T_{F(y)}$, because the map F is assumed to be immersion, that is the differential $(D_y F)$ is the isomorphism onto the tangent space $T_{F(y)}$.

The main focus of our analysis is the *invariance equation*[1]:

$$\Delta = (1 - P)J = 0 \,,$$

the *defect of invariance* Δ should vanish. It is a differential equation for an unknown map $F : W \to U$. Solutions of this equation are invariant in the sense that the vector field $J(x)$ is tangent to the manifold $\Omega = F(W)$ for

[1] A.M. Lyapunov studied analytical solutions of similar equations near a fixed point [3]. He found these solutions in a form of the Taylor series expansion and proved the convergency of those power series near the non-resonant fixed point (the Lyapunov auxiliary theorem). In 1960s the invariance equations approach was developed, first of all, in the context of the Kolmogorov–Arnold–Moser theory for invariant tori computation [4–6], as a special analytical perturbation theory [7,8]. Recently, the main task is to develop constructive non-perturbative methods, because the series of perturbations theory diverge and, moreover, the high–order terms loose the physical sense for most interesting applications. The seminal Kolmogorov's idea was to use Newton's method for solution of the invariance equation (instead of the Taylor series expansion) [4]. In this book we discuss the methods for invariant manifold construction that exploit the thermodynamic properties of the kinetic equations.

each point $x \in \Omega$. But this condition says nothing about the slowness of the manifold Ω.

How to choose the projector P? Another form of this question is: how to define the plain of fast motions $x + \ker P$? The choice of the projector P is ambiguous, from the formal point of view, but the second law of thermodynamics gives a good hint [9]: the entropy should grow in the fast motion, and the point x should be the point of entropy maximum on the plane of fast motion $x + \ker P$. That is, the subspace $\ker P$ should belong to the kernel of the entropy differential:

$$\ker P_x \subset \ker D_x S \ .$$

Of course, this rule is valid for closed systems with entropy, but it can be also extended onto open systems: the projection of the "thermodynamic part" of $J(x)$ onto T_x should have the positive entropy production. If this thermodynamic requirement is valid for any ansatz manifold not tangent to the entropy levels and for any thermodynamic vector field, then the thermodynamic projector is unique [10]. Let us describe this projector P for given point x, subspace $T_x = \mathrm{imP}$, differential $D_x S$ of the entropy S at the point x and the second differential of the entropy at the point x, the bilinear functional $(D_x^2 S)_x$. We need the positively definite bilinear form $\langle z|p\rangle_x = -(D_x^2 S)_x(z,p)$ (the entropic scalar product). There exists a unique vector g such that $\langle g|p\rangle_x = D_x S(p)$. It is the Riesz representation of the linear functional $D_x S$ with respect to entropic scalar product. If $g \neq 0$ then the thermodynamic projector is

$$P(J) = P^{\perp}(J) + \frac{g^{\|}}{\langle g^{\|}|g^{\|}\rangle_x}\langle g^{\perp}|J\rangle_x \ ,$$

where $P^{\perp}$ is the orthogonal projector onto T_x with respect the entropic scalar product, and the vector g is splitted onto tangent and orthogonal components:

$$g = g^{\|} + g^{\perp};\ g^{\|} = P^{\perp}g;\ g^{\perp} = (1 - P^{\perp})g \ .$$

This projector is defined if $g^{\|} \neq 0$.

If $g = 0$ (the equilibrium point) then $P(J) = P^{\perp}(J)$.

For given T_x, the *thermodynamic projector* (5.25) depends on the point x through the x-dependence of the scalar product $\langle|\rangle_x$, and also through the differential of S in x.

A dissipative system may have many closed positively invariant sets. For example, for every set of initial conditions K, union of all the trajectories $\{x(t), t \geq 0\}$ with initial conditions $x(0) \in K$ is positively invariant. Thus, the selection of the slow (stable) positively invariant manifolds becomes an important problem[2].

[2] Nevertheless, there exists a different point of view: "Non–uniqueness, when it arises, is irrelevant for modeling" [13], because the differences between the possible manifolds are of the same order as the differences we set out to ignore in

One of the difficulties in the problem of reducing the description is due to the fact that there exists no commonly accepted formal definition of a slow (and stable) positively invariant manifold. This difficulty is resolved in Chap. 4 of our book in the following way: First, we consider manifolds immersed into a phase space and study their motion along trajectories. Second, we subtract from this motion the motion of immersed manifolds along themselves, and obtain a new equation for dynamics of manifolds in the phase space: the manifold Ω moves by the vector field Δ. It is *the film extension of the dynamics*:

$$\frac{\mathrm{d}F_t(y)}{\mathrm{d}t} = \Delta \,,$$

where the defect of invariance, $\Delta = (1-P)J$, depends on the point $x = F(y)$ and on the tangent space to the manifold $\Omega = F(W)$ at this point. Invariant manifolds are fixed points for this extended dynamics, and *slow* invariant manifolds are *Lyapunov stable fixed points*.

The main body of this book is about how to actually compute the slow invariant manifold. We present three approaches to constructing slow (stable) positively invariant manifolds.

- *Iteration method* for solution of the invariance equation (Newton method subject to incomplete linearization);
- *Relaxation methods* based on the film extension of the original dynamic system;
- *The method of natural projector* that projects not the vector fields, but rather finite segments of trajectories.

The Newton method (with incomplete linearization) is the iteration method for solving the invariance equation. On each iteration we linearize the invariance equation and solve obtained linear equation. In the defect of invariance $\Delta = (1-P)J(x)$ both the vector field $J(x) = J(F(y))$ $(y \in W)$ and the projector P depend on the unknown map F (P depends on the point $x \in W$ and on the tangent space $T_x = \mathrm{im}D_yF$). On each iteration we use for $J(F(y))$ the first-order (linear in F) approximation, and for P only the zero-order (constant) one. The iteration method with this *incomplete linearization* leads to the slowest invariant manifold [11]. The Newton method (with incomplete linearization) is convenient for obtaining the explicit formulas – even one iteration can give a good approximation.

Relaxation methods are directed more towards the numerical implementation. Nevertheless, several first steps also can give appropriate analytical approximations, competitive with other methods. These methods are based on the stepwise solution of the differential equation $\mathrm{d}F(y)/\mathrm{d}t = \Delta$ (the *film extension of the dynamics*).

---

establishing the low-dimensional model. We do not share this viewpoint because it may be relevant only if there exists a small parameter, and, moreover, only asymptotically when this small parameter tends to zero.

Finally, the natural projector method constructs not the manifold itself but a projection of slow dynamics onto some set of variables. This method is the successor of two important methods: the Ehrenfests' coarse-graining [15] and the Hilbert method for solution of the Boltzmann equation [16]. It can by applied to reversible and irreversible systems, and allows us to make the first step of reduction (see Fig. 1.1) as well as the following steps.

The Newton method subject to incomplete linearization was developed for the construction of slow (stable) positively invariant manifolds in the following problems:

- Derivation of the post–Navier–Stokes hydrodynamics from the Boltzmann equation [11, 12, 14, 17].
- Description of the dynamics of polymers solutions [12, 106].
- Correction of the moment equations [12, 21].
- Reduced description for chemical kinetics [12, 22, 23, 105].

Relaxation methods based on the film extension of the original dynamic system were applied to the Fokker–Planck equation [12, 24]. Applications of these methods in the theory of the Boltzmann equation can benefit from the estimations, obtained in the papers [26, 27].

The method of natural projector was originally applied to derivation of the dissipative equations of macroscopic dynamics from the conservative equations of the microscopic dynamics [12, 29–35]. Using this method, new equations were obtained for the post–Navier–Stokes hydrodynamics, equations of plasma hydrodynamics and others [30, 34]. This short-memory approximation was applied to the Wigner formulation of quantum mechanics [36–38]. The dissipative dynamics of a single quantum particle in a confining external potential is shown to take the form of a damped oscillator whose effective frequency and damping coefficients depend on the shape of the quantum-mechanical potential [35]. Further examples of the coarse-graining quantum fields dynamics can be found in [39]. The natural projector method can also be applied effectively to dissipative systems: instead of the Chapman–Enskog method in theory of the Boltzmann equation, for example.

The most natural initial approximation for the methods under consideration is a quasiequilibrium manifold. It is the manifold of conditional maxima of the entropy. The majority of works on nonequilibrium thermodynamics deal with corrections to quasi-equilibrium approximations, or with applications of these approximations (with or without corrections). The construction of the quasi-equilibrium allows for the following generalization: almost every manifold can be represented as a set of minimizers of the entropy under linear constraints. However, in contrast to the standard quasiequilibrium, these linear constraints will depend on the point on the manifold. We describe the quasiequilibrium manifold and the quasiequilibrium projector on the tangent space of this manifold. This projector is orthogonal with respect to the entropic scalar product (the bilinear form defined by the negative second differential of the entropy). We construct the thermodynamical projector, which

transforms the arbitrary vector field equipped with the given Lyapunov function (the entropy) into a vector field with the same Lyapunov function for an arbitrary anzatz manifold which is not tangent to the level of the Lyapunov function. The uniqueness of this construction is demonstrated.

Here, a comment on the status of most of the statements in this book is in order. Just like the absolute majority of claims concerning such things as general solutions of the Navier–Stokes or the Boltzmann equation, they have the status of being plausible. They can become theorems only if one restricts essentially the set of the objects under consideration. Among such restrictions we should mention cases of the exact reduction, for example, exact derivation of hydrodynamics from kinetics [40, 42]. In these (still infinite-dimensional) examples one can compare different methods, for example, the Newton method with the methods of series summation in the perturbation theory [42, 43].

Also, it is necessary to stress here, that even if in the limit all the methods lead to the same results, they can give rather different approximations "on the way".

The rigorous foundation of the constructive methods of invariant manifolds should, in particular, include theorems about *persistence of invariant manifolds under perturbations*. For instance, the compact normally hyperbolic invariant manifolds persist under small perturbations for finite-dimensional dynamical systems [46, 47]. The most well-known result of this type is the Kolmogorov–Arnold–Moser theory about persistence of almost all invariant tori of completely integrable system under small perturbations [4–6].

Such theorems exist for some classes of infinite dimensional dissipative systems too [48]. Unfortunately, it is not proven until now that many important systems (the Boltzmann equation, the three-dimensional Navier–Stokes equations, the Grad equations, etc.) belong to these classes. So, it is necessary to act with these systems without a rigorous basis.

The new quantum field theory formulation of the problem of persistence of invariant tori in perturbed completely integrable systems was obtained [68], and a new proof of the KAM theorem for analytic Hamiltonians based on the renormalization group method was given.

Two approaches to the construction of the invariant manifolds are widely used: the *Taylor series expansion* for the solution of the invariance equation [3, 50–52] and the method of *renormalization group* [53, 54, 56–59]. The advantages and disadvantages of the Taylor series expansion are well-known: constructivity versus the absence of physical meaning for the high-order terms (often), and divergence in the most interesting cases (often).

In the paper [56], a geometrical formulation of the renormalization group method for global analysis was given. It was shown that the renormalization group equation can be interpreted as an envelope equation. Recently [57] the renormalization group method was formulated in terms of invariant manifolds. This method was applied to derive kinetic and transport equations from

the respective microscopic equations [58]. The derived equations include the Boltzmann equation in classical mechanics (see also the paper [55], where it was shown for the first time that kinetic equations such as the Boltzmann equation can be understood naturally as renormalization group equations), the Fokker–Planck equation, a rate equation in a quantum field theoretical model.

From the point of view of the authors of the paper [55], the relation of renormalization group theory and reductive perturbation theory has simultaneously been recognized: renormalization group equations are actually the slow-motion equations which are usually obtained by reductive perturbation methods.

The renormalization group approach was applied to the stochastic Navier–Stokes equation in order to model fully developed fluid turbulence [60–62]. For the evaluation of the relevant degrees of freedom the renormalization group technique was revised for discrete systems in the recent paper [59].

The kinetic theory approach to subgrid modeling of fluid turbulence became more popular recently. [63–66]. A mean-field approach (filtering out subgrid scales) was applied to the Boltzmann equation in order to derive a subgrid turbulence model based on kinetic theory. It was demonstrated [66] that the only Smagorinsky type model which survives in the hydrodynamic limit on the viscosity time scale is the so-called tensor-diffusivity model [67].

The first systematic and successful method of constructing invariant manifolds for dissipative systems was the celebrated *Chapman-Enskog method* [70] for the Boltzmann kinetic equation. The Chapman–Enskog method results in a series development of the so-called normal solution (the notion introduced by Hilbert [16]) where the one-body distribution function depends on time and space only through its locally conserved moments. To the first approximation, the Chapman–Enskog method leads to hydrodynamic equations with transport coefficients expressed in terms of molecular scattering cross-sections. However, the higher order terms of the Chapman–Enskog expansion bring in the "ultra-violet catastrophe" (noticed first by Bobylev [72]) and negative viscosity. This drawback pertinent to the Taylor series expansion disappears as soon as the Newton method is used to construct the invariant manifold [11].

The Chapman–Enskog method was generalized many times [76] and gave rise to a host of subsequent works and methods, such as the famous method of the *quasi-steady state* in chemical kinetics, pioneered by Bodenstein and Semenov and explored in considerable detail by many authors (see, for example, [22, 77–81]), and the theory of *singularly perturbed* differential equations [77, 82–87].

There exists a set of methods to construct an ansatz for the invariant manifold based on the spectral decomposition of the Jacobian. The idea to use the spectral decomposition of Jacobian fields in the problem of separating the motions into fast and slow originates from analysis of stiff systems [88],

and from methods of sensitivity analysis in control theory [89, 90]. One of the currently most popular methods based on the spectral decomposition of Jacobian fields is the construction of the so-called *intrinsic low-dimensional manifold* (ILDM) [93].

These methods were thoroughly analyzed in two papers [94, 95]. It was shown that the successive applications of the Computational Singular Perturbation (CSP) algorithm (developed in [90]) generate, order by order, the asymptotic expansion of a slow manifold, and the manifold identified by the ILDM technique (developed in [93]) agrees with the invariant manifold to some order. An explicit algorithm based on the CSP method is designed for the integration of stiff systems of PDEs by means of explicit schemes [91]. The CSP analysis of time scales and manifolds in a transient flame-vortex interaction was presented in [92].

The theory of *inertial manifold* is based on the special linear dominance in higher dimensions. Let an infinite-dimensional system have a form: $\dot{u} + Au = R(u)$, where A is self-adjoint, and has a discrete spectrum $\lambda_i \to \infty$ with sufficiently big gaps between λ_i, and let $R(u)$ be continuous. One can build the slow manifold as the graph over a root space of A [96]. The textbook [100] provides an exhaustive introduction to the main ideas and methods of this theory. Systems with linear dominance have limited utility in kinetics. Often there are no big spectral gaps between λ_i, and even the sequence $\lambda_i \to \infty$ might be bounded (for example, this is the case for the model Bhatnagar–Gross–Krook (BGK) equations, or for the Grad equations). Nevertheless, the concept of the inertial attracting manifold has wider field of applications than the theory, based on the linear dominance assumption.

The Newton method with incomplete linearization and the relaxation method allow us to find an approximate slow invariant manifolds without Jacobian field spectral decomposition. Moreover, a necessary slow invariant subspace of the Jacobian at the equilibrium point appears as a by-product of the Newton iterations (with incomplete linearization), or of the relaxation method.

It is of importance to search for minimal (or subminimal) sets of natural parameters that uniquely determine the long-time behaviour of a system. This problem was first discussed by Foias and Prodi [97] and by Ladyzhenskaya [98] for the two-dimensional Navier–Stokes equations. They have proved that the long-time behaviour of solutions is completely determined by the dynamics of sufficiently large number of Fourier modes. A general approach to the problem on the existence of a finite number of determining parameters has been discussed [99, 100].

The past decade has witnessed a rapid development of the so-called *set oriented* numerical methods [101]. The purpose of these methods is to compute attractors, invariant manifolds (often, computation of stable and unstable manifolds in hyperbolic systems [102–104]). Also, one of the central tasks of these methods is to gain statistical information, i. e. computations

of physically observable invariant measures. The distinguished feature of the modern set-oriented methods of numerical dynamics is the use of ensembles of trajectories within a relatively short propagation time instead of a long time single trajectory.

In this book we systematically consider a discrete analog of the slow (stable) positively invariant manifolds for dissipative systems, *invariant grids*. These invariant grids were introduced in [22]. Here we shall describe the Newton method subject to incomplete linearization and the relaxation methods for the invariant grids [105].

It is worth mentioning that the problem of the grid correction is fully decomposed into the tasks of the grid's nodes correction. The edges between the nodes appear only in the calculation of the tangent spaces at the nodes. This fact determines the high computational efficiency of the invariant grids method.

Let the (approximate) slow invariant manifold for a dissipative system be found. *Why have we constructed it?* One important part of the answer to this question is: *We have constructed it to create models of open system dynamics in the neighborhood of this manifold*. Different approaches for this modeling are described.

We apply these methods to the problem of reduced description in polymer dynamics and derive the universal limit in dynamics of dilute polymeric solutions. It is represented by the *revised Oldroyd 8 constants* constitutive equation [106] for the polymeric stress tensor. Coefficients of this constitutive equation are expressed in terms of the microscopic parameters. This limit of dynamics of dilute polymeric solutions is universal, and any physically consistent equation should contain the obtained equation as a limit, or one should explain why it is not achieved. Such universal limit equations are well-known in various fields of physics. For example, the Navier–Stokes equation in fluid dynamics is an universal limit for dynamics of simple gas described by the Boltzmann equation, the Korteweg–De-Vries equation is universal in the description of the dispersive dissipative nonlinear waves, etc.

The phenomenon of *invariant manifold explosion* in driven open systems is demonstrated on the example of dumbbell models of dilute polymeric solutions [109]. This explosion gives us a possible mechanism of drag reduction in dilute polymeric solutions [110].

Suppose that for the kinetic system the approximate invariant manifold has been constructed and the slow motion equations have been derived. Suppose that we have solved the slow motion system and obtained $x_{sl}(t)$. We consider the following two questions:

- How well does this solution approximate the true solution $x(t)$ given the same initial conditions?
- How is it possible to use the solution $x_{sl}(t)$ for its refinement without solving the slow motion system (or its modifications) again?

These two questions are interconnected. The first question states the problem of the *accuracy estimation*. The second one states the problem of *post-processing* [348–351]. We propose various algorithms for post-processing and accuracy estimation, and give an example of application.

Our collection of methods and algorithms can be incorporated into recently developed technologies of computer-aided multiscale analysis which enable "level jumping" between microscopic and macroscopic (system) levels. It is possible both for the traditional technique based on transition from microscopic equations to macroscopic equations and for the "equation-free" approach [107]. This approach developed in recent work [108], when successful, can bypass the derivation of the macroscopic evolution equations when these equations conceptually exist but are not available in closed form. The mathematics-assisted development of a computational superstructure may enable alternative descriptions of the problem physics (e.g. Lattice Boltzmann (LB), kinetic Monte- Carlo (KMC) or Molecular Dynamics (MD) microscopic simulators, executed over relatively short time and space scales) to perform systems level tasks (integration over relatively large time and space scales, coarse bifurcation analysis, optimization, and control) directly. It is possible to use macroscopic invariant manifolds in this environment without explicit equations.

1.2 Content and Reading Approaches

The present book comprises sections of two kinds. The first includes the sections that contain basic notions, methods and algorithms. Another group of sections entitled "Examples" contain various case studies where the methods are applied to specific equations. Exposition in the "Examples" sections is not as consequent as in the basic sections. Most of the examples can be read more or less independently. Logical connections between chapters are presented in Fig. 1.3.

The main results and notions presented in the book are as follows. In this Chap. 1 we present the main ideas, references, abstracts of chapters, and the possible reading plans.

Chapter 2 is the second introduction, it introduces the main equations of kinetics: the Boltzmann equation, equations of chemical kinetics, and the Fokker–Planck equation. The main methods of reduction for these equations are also discussed: from the Chapman–Enskog and Hilbert methods to quasiequilibrium and quasi-steady state approximations.

In Chap. 3 we write down the *invariance equation* in the differential form. This equation gives the necessary conditions of invariance of a manifold immersed into the phase space of a dynamical system. In order to estimate the discrepancy of an ansatz manifold, the *defect of invariance* if defined. The introduction of this defect of invariance requires a *projector field*. These

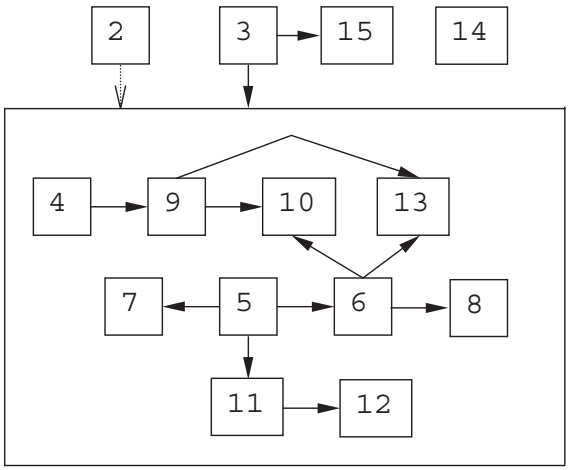

Fig. 1.3. Logical connections between chapters. All the chapters depend on Chap. 3. For understanding examples and problems it may be useful (but not always necessary) to read Chap. 2

notions, defect of invariance and projector field, as well as the invariance equation play the central role in the whole book.

Chapter 4 is devoted to the definition of *slowness* of a positively invariant manifold. The equation of motion of the manifold (the "film") immersed into the phase space of the dynamical system is discussed (equation for the film motion). A slow positively invariant manifold is defined as a stable fixed point for this motion. The projector field introduced in Chap. 3 is crucial for the definition of the stability.

The main thermodynamic structures, the entropy, the entropic scalar product, quasiequilibrium, and the thermodynamic projector, are introduced in Chap. 5. The quasiequilibrium manifold is the manifold of conditional entropy maxima for given values of macroscopic variables. These values parametrize this manifold. Most of the works on nonequilibrium thermodynamics deal with corrections to quasiequilibrium approximations, or with applications of these approximations (with or without corrections). This viewpoint is not the only possible, but it proves very efficient for the construction of a variety of useful models, approximations and equations, as well as methods to solve them.

The entropic scalar product is generated by the second differential of the entropy. It endows the space of states by the unique distinguished Riemannian structure. The thermodynamic projector is the operator which transforms the arbitrary vector field equipped with the given Lyapunov function into a vector field with the same Lyapunov function. Uniqueness of such projector is proved.

In Chap. 5 we start the series of examples for the Boltzmann equations. First, we analyze the defect of invariance for the Local Maxwellian manifold: the manifold of the locally equilibrium distributions. Second, we present the quasi-equilibrium closure hierarchies for the Boltzmann equation. In 1949, Harold Grad [201] extended the basic assumption behind the Hilbert and Chapman–Enskog methods (the space and time dependence of the normal solutions is mediated by the five hydrodynamic moments). A physical rationale behind the Grad moment method is an assumption of the decomposition of motion. (i) During the time of order τ, a set of distinguished moments M' (which include the hydrodynamic moments and a subset of higher-order moment) does not change significantly as compared to the rest of the moments M'' (the fast evolution). (ii) Towards the end of the fast evolution, the values of the moments M'' become unambiguously determined by the values of the distinguished moments M'. (iii) On the time of order $\theta \gg \tau$, dynamics of the distribution function is determined by the dynamics of the distinguished moments while the rest of the moments remains to be determined by the distinguished moments (the slow evolution period).

An important generalization of the Grad moment method is the concept of quasiequilibrium approximations. The quasiequilibrium distribution function for a set of distinguished moments M' maximizes the entropy density S for fixed M'. The quasiequilibrium manifold is the collection of the quasiequilibrium distribution functions for all admissible values of M. The quasiequilibrium approximation is the simplest and very useful (not only in the kinetic theory itself) implementation of the hypothesis about time separation.

The quasiequilibrium approximation does not exist if the highest order moment is an odd polynomial of velocity (therefore, there exists no quasiequilibrium for thirteen Grad's moments). The Grad moment approximation is the first-order expansion of the quasiequilibrium around the local Maxwellian. An explicit method of constructing of approximations (the Triangle Entropy Method) is developed for strongly nonequilibrium problems of Boltzmann–type kinetics, i.e. when standard moment variables are insufficient. This method enables one to treat any complicated nonlinear functionals that fit the physics of a problem (such as, for example, rates of processes) as new independent variables.

The method is applied to the problem of derivation of hydrodynamics from the Boltzmann equation. New macroscopic variables are introduced (moments of the Boltzmann collision integral, or collision moments). They are treated as independent variables rather than as infinite moment series. This approach gives the complete account of the rates of scattering processes. Transport equations for scattering rates are obtained (the second hydrodynamic chain), similar to the usual moment chain (the first hydrodynamic chain). Using the triangle entropy method, three different types of macroscopic description are considered. The first type involves only moments of

distribution functions, and the results coincide with those of the Grad method in the Maximum Entropy version. The second type of description involves only collision moments. Finally, the third type involves both the moments and the collision moments (the mixed description). The second and the mixed hydrodynamics are sensitive to the choice of the collision model. The second hydrodynamics is equivalent to the first hydrodynamics only for Maxwell molecules, and the mixed hydrodynamics exists for all types of collision models excluding Maxwell molecules. Various examples of the closure of the first, of the second, and of the mixed hydrodynamic chains are considered for the hard spheres model. It is shown, in particular, that the complete account of scattering processes leads to a renormalization of transport coefficients.

We apply the developed method to a classical problem: determination of molecular dimensions (as diameters of equivalent hard spheres) from experimental viscosity data. It is the third example in Chap. 5.

The first non-perturbative method for solution of the invariance equation is developed in Chap. 6. It is the *Newton method with incomplete linearization*. The incomplete linearization means that in the Newton–type iteration for the invariance equation we do not use the whole differential of the right-hand side of the invariance equation: the differential of the projector field is excluded. This modification of the Newton method leads to selection of the slowest invariant manifold. The series of examples for the Boltzmann equations is continued in this chapter. The non-perturbative correction to the Local Maxwellian manifold is constructed, and the equations of the high-order (the post–Navier–Stokes) hydrodynamics are obtained.

In Chap. 5 we use the second law of thermodynamics – existence of the entropy – in order to equip the problem of constructing slow invariant manifolds with a geometric structure. The requirement of the entropy growth (universally, for all the reduced models) significantly restricts the form of the thermodynamic projectors. In Chap. 7 we introduce a different but equally important argument – the *micro-reversibility* (T-invariance), and its macroscopic consequences, the *Onsager reciprocity relations*. The main idea in this chapter is to use the reciprocity relations for the fast motions. In order to appreciate this idea, we should mention that the decomposition of motions into fast and slow is not unique. Requirement of the Onsager reciprocity relations for any equilibrium point of fast motions implies the selection (filtration) of the fast motions. We term this the *Onsager filter*. Equilibrium points of fast motions are all the points on manifolds of slow motions. The formalism of the *quasi-chemical representation* is one of the most developed means of modelling, it makes it possible to "assemble" complex processes out of elementary processes. This formalism is very natural for representation of the reciprocity relations. And again, the Example to this chapter continues the "Boltzmann series". It is the quasi-chemical representation and the self-adjoint (i.e. Onsager) linearization of the Boltzmann collision operator in the slow, but not obligatory equilibrium states.

In Chap. 8 a new class of exactly solvable problems in nonequilibrium statistical physics is described. The systems that allow the exact solution of the reduction problem are presented. Up to now, the problem of the exact relationship between kinetics and hydrodynamics remains unsolved. All the methods used to establish this relationship are not rigorous, and involve approximations. In this chapter, we consider situations where hydrodynamics is the exact consequence of kinetics, and in that respect, a new class of exactly solvable models of statistical physics has been established. The Chapman–Enskog method is treated as the Taylor series expansion approach to solving the appropriate invariance equation. A detailed treatment of the classical Chapman–Enskog derivation of hydrodynamics is given in the framework of Grad's moment equations. Grad's systems are considered as the minimal kinetic models where the Chapman–Enskog method can be studied exactly, thereby providing the basis to compare various approximations in extending the hydrodynamic description beyond the Navier–Stokes approximation. Various techniques, such as the method of partial summation, the Padé approximants, and the invariance principle are compared both in linear and nonlinear situations.

In Chap. 9 the "large stepping" *relaxation method* for solution of the invariance equation is developed. The relaxation method is an alternative to the Newton iteration method described in Chap. 6: The initial approximation to the invariant manifold is moved with the film extension of the dynamics described in Chap. 4. The proposed step in time for the stepwise solution of the film extension equation is the maximal possible step that does not violate the thermodynamic conditions. In the examples, the idea of the large stepping is applied to the Fokker–Planck equation and to the initial layer problem for the Boltzmann equation. The obtained approximate solutions of the initial layer problem are compared to the exact solutions.

How can we represent invariant manifolds numerically? How can we use the numerical representation in all the methods for invariant manifold refinement? Chapter 10 is devoted to answering these questions. A grid-based version of the method of invariant manifold is developed. The most essential element of this chapter is the systematic consideration of a discrete analogue of the slow (stable) positively invariant manifolds for dissipative systems, *invariant grids*. The invariant grid is defined as a mapping of finite-dimensional grids into the phase space of a dynamic system. We define the differential operators on the grid as difference operators, hence, it is possible to define the tangent space at each point of the grid mapped into the phase space. If the tangent space is constructed, then the invariance equation can be written down. We describe the Newton method and the relaxation method for solution of this discrete analogue of the invariance equation. Examples for this chapter are taken from the chemical kinetics. One attractive feature of two-dimensional invariant grids is the possibility to use them as a screen, on which one can display different functions and dynamic of the system.

P. and T. Ehrenfest suggested in 1911 a model of dynamics with a coarse-graining of the original conservative system in order to introduce irreversibility [15]. The Ehrenfests considered a partition of the phase space into small cells, and they have suggested combining the motions of the phase space ensemble due to the Liouville equation with coarse-graining "shaking" steps – averaging of the density of the ensemble over the phase cells. This generalizes to the following: combination of the motion of the phase ensemble due to microscopic equations with returns to the quasiequilibrium manifold while preserving the values of the macroscopic variables. In Chap. 11 we develop the method of natural projector, a formalism of nonequilibrium thermodynamics based on this generalization.

The method of natural projector can be considered as a development of the ideas of the Hilbert method from the theory of the Boltzmann equation. The main new element in the method of natural projector with respect to the Hilbert method is the construction of the macroscopic equations from the microscopic equations, not just a "normal solution" to a microscopic equation. The obtained macroscopic equations contain one unknown parameter, the time between coarse-graining (shaking) steps (τ). This parameter can be obtained from the experimental data, or from independent microscopic or phenomenological consideration.

In the first example to this chapter the microscopic dynamics is given by the one-particle Liouville equation. The set of macroscopic variables is density, momentum density, and the density of average kinetic energy. The correspondent quasiequilibrium distribution is the local Maxwell distribution. For the hydrodynamic equations, the zeroth (quasiequilibrium) approximation is given by the Euler equations of compressible nonviscous fluid. The next order approximation gives the Navier–Stokes equations which have dissipative terms. Higher-order approximations to the hydrodynamic equations, when they are derived from the Boltzmann kinetic equation by the Chapman–Enskog expansion (so-called Burnett approximation), are prone to various difficulties, in particular, they exhibit instability of sound waves at sufficiently short wave length (see Chap. 8). Here we demonstrate how model hydrodynamic equations, including the post–Navier–Stokes approximations, can be derived on the basis of the coarse-graining idea, and find that the resulting equations are stable, contrary to the Burnett equation.

In the second example the fluctuation-dissipation formula is derived by the method of natural projector and is illustrated by the explicit computation for the exactly solvable McKean kinetic model [285]. It is demonstrated that the result is identical, on the one hand, to the sum of the Chapman–Enskog expansion, and, on the other hand, to the exact solution of the invariance equation.

In Chap. 12 the general geometrical framework of nonequilibrium thermodynamics is developed. It is the generalization of the method of natural projector (Chap. 11) to large steps in time. The notion of *macroscopically*

definable ensembles is introduced. The thesis about macroscopically definable ensembles is suggested. This thesis should play the same role in the nonequilibrium thermodynamics, as the Church–Turing thesis in the theory of computability. The *primitive macroscopically definable ensembles* are described. These are ensembles with macroscopically prepared initial states.

The method for computing trajectories of primitive macroscopically definable nonequilibrium ensembles is elaborated. These trajectories are represented as sequences of deformed equilibrium ensembles and simple quadratic models between them. The primitive macroscopically definable ensembles form a manifold in the space of ensembles. We call this manifold the *film of nonequilibrium states*. The equation for the film and the equation for the ensemble motion on the film are written down. The notion of the invariant film of non-equilibrium states, and the method of its approximate construction transform the problem of nonequilibrium kinetics into a series of problems of equilibrium statistical physics. The developed methods allow us to solve the problem of macro-kinetics even when there are no autonomous equations of macro-kinetics.

The slow invariant manifold for a closed system has been found. What next? Chapter 13 gives the answer to this question. The theory of invariant manifolds is developed for weakly open systems. In the first example the method of invariant manifold for driven systems is developed for a derivation of a reduced description in kinetic equations of dilute polymeric solutions. The method applies to any models of polymers and is consistent with basic physical requirements: frame invariance and dissipativity of resulting constitutive equation. It is demonstrated that this reduced description becomes universal in the limit of small Deborah and Weissenberg numbers, and it is represented by the *revised Oldroyd 8 constants constitutive equation* for the polymeric stress tensor. This equation differs from the classical Oldroyd 8 constants constitutive equation by one additional term. Coefficients of this constitutive equation are expressed in terms of the microscopic parameters of the polymer model. A systematic procedure of corrections to the revised Oldroyd 8 constants equations is developed. Results are tested with simple flows.

In the second example in this chapter the derivation of macroscopic equations from the simplest dumbbell models is revisited. It is demonstrated that the onset of the macroscopic description is sensitive to the flows. For the FENE-P model it is shown that there is a possibility of "explosion" of the Gaussian manifold: with a small initial deviation, solution of the kinetic equation very quickly deviate from the manifold, and then slowly come back to the stationary point located on the Gaussian manifold. Nevertheless, the Gaussian manifold remains invariant. Some consequences of these observations are discussed. A new class of closures is introduced, the kinetic multipeak polyhedra. Distributions of this type are expected in kinetic models with multidimensional instability as universally, as the Gaussian distribution

appears for stable systems. The number of possible relatively stable states of a nonequilibrium system grows as 2^m, and the number of macroscopic parameters is of the order mn, where n is the dimension of configuration space, and m is the number of independent unstable directions in this space. The elaborated class of closures and equations pretends to describe the effects of so-called "molecular individualism".

How can we prove that all the attractors of a infinite-dimensional system belong to a finite-dimensional manifold? How can we estimate the dimension of this manifold? There are two methods for such estimations, discussed in Chap. 14. First, if we find that *k-dimensional volumes are contracted* due to dynamics, then (after some additional technical steps concerning existence of the positively–invariant bounded set and uniformity of the k-volume contraction on this set) we can state that the *Hausdorff dimension* of the maximal attractor is less, then k. Second, if we find the representation of our system as a nonlinear kinetic system with *conservation of supports* of distributions, then (again, after some additional technical steps) we can state that the asymptotics is finite-dimensional. This conservation of support has a *quasi-biological interpretation, the inheritance* (if a gene is not presented in an isolated population without mutations, then it cannot appear in time). The finite-dimensional asymptotics demonstrates the effects of *"natural" selection*.

The post-processing (Chap. 15) is a very simple, but attractive idea. In the method of invariant manifold we improve the whole manifold on each iteration. If we need only one or several solutions, this whole manifold may be too big for our goals, and we can restrict our activity by refinement of a given solution: a curve instead of a multi-dimensional manifold. The classical Picard iteration for a solution of a differential equation gives the simplest post-processing. Various forms of post-processing are presented. In the example to this chapter the method which recognizes the onset and breakdown of the macroscopic description in microscopic simulations is presented. The method is based on the invariance of the macroscopic dynamics relative to the microscopic dynamics, and it is demonstrated for a model of dilute polymeric solutions where it decides switching between Direct Brownian Dynamics simulations and integration of constitutive equations.

The list of cited literature is by no means complete although we spent effort in order to reflect at least the main directions of studies related to computations of the invariant manifolds. We think that this list is more or less exhaustive in the second-order approximation.

There are many different roads of reading this book. Chapter 3 is necessary for reading all of the other chapters, as is shown in the flowchart (Fig. 1.3). Here we propose several possible roads. This is not the exhaustive list, and everybody can invent his own road.

The *short formal road*: Chap. 3, Sects.: 4.1, 5.1–5.3, 6.1, 7.1, 9.1, 10.1, 11.1, 13.1–13.4, 15.1. If you are ready to look at the formal ordinary differential

equation $\frac{\mathrm{d}x}{\mathrm{d}t} = J(x),\ x \in U$, and to imagine in this form all the kinetic equations, from the Boltzmann equation to the Fokker–Planck equation, then this formal road is the best way to start. After that, you can choose various examples and chapters. Before reading the examples sections, it may be useful to look through Chap. 2.

The *long formal road*: Chaps. 3, 4, Sects.: 5.1–5.3, 6.1, 7.1, 9.1, 10.1, 11.1, 13.1–13.4, 14.1, 14.2, 15.1.

The *short Boltzmann road*: Chap. 2 (including chemical kinetics), Chap. 3, Sects. 5.1–5.3, 5.5, 6.1–6.3, Chap. 8. This road gives the invariance equation, the Newton method with incomplete linearization for solution of this equation, the theory of Local Maxwellian manifold, and the application of this method to correction of these manifolds. Chapter 8 adds the exact solutions of the reduction problem and the test of the developed methods on these solutions.

The *long Boltzmann road*: Chap. 2 (including chemical kinetics), Chap. 3, Sects. 5.1–5.3, 5.5, 5.6, 5.7, Chaps. 6–8, Sects. 4.1, 9.1, 9.3. Exhaustive reading: everything concerning the Boltzmann equation.

The *nonequilibrium thermodynamic road*: Chap. 2, Chap. 3, Sects. 4.1, 5.1–5.4, 7.1, 9.1, Chaps. 11, 12, 14. This road can be naturally supplemented by some sections from the Boltzmann roads.

The *short Grad road*: Chaps. 2, 3, Sects. 5.1–5.6, 6.1, Chap. 8.