3 Invariance Equation in Differential Form

Definition of invariance in terms of motions and trajectories assumes, at least, existence and uniqueness theorems for solutions of the original dynamical system. This prerequisite causes difficulties when one studies equations relevant to physical and chemical kinetics, such as, for example, equations of hydrodynamics. Nevertheless, there exists a necessary *differential condition of invariance*: The vector field of the original dynamic system touches the manifold at every point. Let us write down this condition in order to set up the notation.

Let E be a linear space, U (the phase space) be a domain in E, and let a vector field $J: U \to E$ be defined in U. This vector field defines the original dynamical system,

$$\frac{\mathrm{d}x}{\mathrm{d}t} = J(x),\ x \in U \ . \tag{3.1}$$

In the sequel, we consider submanifolds in U which are parameterized by a given set of parameters. Let a linear space of parameters L be defined, and let W be a domain in L. We consider differentiable maps, $F: W \to U$, such that, for every $y \in W$, the differential of F, $D_yF: L \to E$, is an isomorphism of L on a subspace of E. That is, F are the manifolds, immersed in the phase space of the dynamical system (3.1), and parametrized by the parameter set W.

Remark: One never discusses the choice of norms and topologies is such a general setting. It is assumed that the corresponding choice is made appropriately in each specific case.

We denote T_y the tangent space at point y, $T_y = (D_yF)(L)$. *The differential condition of invariance* has the following form: For every $y \in W$,

$$J(F(y)) \in T_y \ . \tag{3.2}$$

Let us rewrite the differential condition of invariance (3.2) in the form of a differential equation. In order to achieve this, one needs to define a projector $P_y: E \to T_y$ for every $y \in W$. Once a projector P_y is defined, then condition (3.2) takes the form:

$$\Delta_y = (1 - P_y)J(F(y)) = 0 \ . \tag{3.3}$$

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Obviously, by $P_y^2 = P_y$ we have, $P_y \Delta_y = 0$. We refer to the function Δ_y as *the defect of invariance* at point y. The defect of invariance will be encountered often in what follows.

Equation (3.3) is the first-order differential equation for the function $F(y)$. Projectors P_y should be tailored to the specific physical features of the problem at hand, and separate chapter below will be devoted to their construction. There we shall demonstrate how to construct a projector, $P(x,T): E \to T$, given a point $x \in U$ and a specified subspace T. We then set $P_y = P(F(y), T_y)$ in equation (3.3)[1].

There are two possible meanings of the notion "approximate solution of the invariance equations" (3.3):

1. Approximation of the solution;
2. The map F with small defect of invariance (the right hand side approximation).

The approximation of the first kind requires theorems about existence of solutions for the initial system (3.1). In order to find this approximation one should estimate the deviations of exact solutions of (3.1) from the approximate invariant manifold. The second kind of approximations does not require the existence of solutions. Moreover, the manifold with sufficiently small defect of invariance can serve as a slow manifold by itself. *The defect of invariance should be small in comparison with the initial vector field J.*

So, we shall accept the concept of approximate invariant manifold (the manifold with small defect of invariance) instead of the approximation of the invariant manifold (see also [25, 349] and other works about approximate inertial manifolds). Sometime these approximate invariant manifolds provide approximations of the invariant manifolds, sometimes not, but it is additional and often difficult problem to make a distinction between these situations. In addition to the defect of invariance, Jacobians, the differentials of $J(x)$, play the key role in the analysis of motion separation into fast and slow. Some estimations of errors of this separation will be presented below in the subsection devoted to *post-processing*.

[1] One of the main routes to define the field of projectors $P(x,T)$ is to make use of a Riemannian structure. To this end, one defines a scalar product in E for every point $x \in U$, that is, a bilinear form $\langle p|q\rangle_x$ with a positive definite quadratic form, $\langle p|p\rangle_x > 0$, if $p \neq 0$. A good candidate for such a scalar product is the bilinear form defined by the negative second differential of the entropy at the point x, $-D^2S(x)$. As we demonstrate later in this book, close to equilibrium this choice is essentially the only correct one. However, far from equilibrium, a refinement is required in order to guarantee the thermodymamicity condition, $\ker P_y \subset \ker(D_xS)_{x=F(y)}$, for the field of projectors, $P(x,T)$, defined for any x and T, if $T \not\subset \ker D_xS$. The thermodymamicity condition provides the preservation of the type of dynamics: if $\mathrm{d}S/\mathrm{d}t > 0$ for initial vector field (3.1) at point $x = F(y)$, then $\mathrm{d}S/\mathrm{d}t > 0$ at this point x for the projected vector field $P_y(J(F(y)))$, too.

Our discussion is focused on nonperturbative methods for computing invariant manifolds, but it should be mentioned that in many applications, the Taylor series expansion is in use, and sometimes works quite well. The main idea is the continuation of the slow manifold with respect to a small parameter: Let our system depend on the parameter ε, and let a manifold of steady states and fibers of motions towards these steady states exist for $\varepsilon = 0$, for example

$$\dot{x} = \varepsilon f(x, y); \;\; \dot{y} = g(x, y) \; . \tag{3.4}$$

For $\varepsilon = 0$, the value of the (vector) variable x is a vector of conserved quantities. Let for every x the equation of fast motion, $\dot{y} = g(x, y)$, be globally stable: Its solution $y(t)$ tends to the unique (for given x) stable fixed point y_x. If the function $g(x, y)$ meets the conditions of the implicit function theorem, then the graph of the map $x \mapsto y_x$ forms a manifold $\Omega_0 = \{(x, y_x)\}$ of steady states. For small $\varepsilon > 0$ we can look for the slow manifold in a form of a series in powers of ε:

$$\Omega_\varepsilon = \{(x, y(x, \varepsilon)\}, \; y(x, \varepsilon) = y_x + \varepsilon y^1(x) + \varepsilon^2 y^2(x) + \dots \; .$$

The fibers of fast motions can be constructed in a form of a power series too (the zero term is the fast motion $\dot{y} = g(x, y)$ in the affine planes $x = \text{const}$). This analytic continuation with respect to the parameter ε for small $\varepsilon > 0$ is studied in the Fenichel's "Geometric singular perturbation theory" [352, 353] (recent applications to chemical kinetics see in [95]). As it was mentioned above, the first successful application of such an approach for the construction of a slow invariant manifold in the form of Taylor series expansion in powers of small parameter ε was the Chapman-Enskog expansion [70].

It is wellknown in various applications that there are many different ways to introduce a small parameter into a system, there are many ways to include a given system in a one-parametric family. Different ways of specification of such a parameter result in different definitions of slowness of positively invariant manifold. Therefore it is desirable to study the notion of separation of motions without such an artificial specification. *The notion of slow positively invariant manifold should be intrinsic.* At least we should try to invent such a notion.