On Conceptual Ideas Concerning Slow Invariant Manifolds in a Variational Problem Viewpoint

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***Abstract*— Chemical combustion models in terms of ordinary differential equations correspond to finite dimensional dissipative dynamical systems involving a multiple time scale structure. A slow mode-description of the full model for dimension reduction purposes can be achieved via computation of stable invariant manifolds. We discuss fundamental and unifying geometric and analytical issues of various approaches to slow invariant manifold computation for model reduction in chemical kinetics and bring up new conceptual ideas concerning the general model reduction problem in terms of slow invariant manifolds with a focus on a variational boundary value problem formulation.**

I. Introduction

Simulation of chemically reacting flows is often nearly impossible in reasonable computing time due to the large number of chemical species involved and the stiffness of the kinetic ordinary differential equations (ODE) with time scales often ranging from nanoseconds to seconds. This calls for multiscale approaches and appropriate model reduction techniques. For this purpose, usually the long time scale system dynamics is approximated via elimination of the fast relaxing modes by enslaving them to the slow ones. In the ideal case, the outcome should be a stable invariant manifold of "slow motion" (SIM) attracting system trajectories from arbitrary initial values. Many model reduction methods use a species reconstruction technique which is provided by an implicitly defined function mapping a subset of the chemical species of the full model – called reaction progress variables (RPVs) – onto the full species composition by determining a point on a SIM.

II. Two basic concepts for slow manifold computation [11]

Finding a functional $\Phi : C^\infty(\mathbb{R}^n) \to \mathbb{R}$ with $\Phi(z) = 0$ that automatically eliminates the fast modes in an ODE model without knowing its analytical solution $z(t) \in \mathbb{R}^n$ explicitly is a general abstract formulation of the main challenge of trajectory-based model reduction approaches. The resulting species reconstruction (SIM computation) problem in chemical kinetics can be formulated as

$$\Phi(z) = 0 \tag{1a}$$
$$\partial_t z(t) = S\left(z(t)\right), \ t \in [t_0, t_\mathrm{f}] \tag{1b}$$
$$z_j(t_\mathrm{f}) = z_j^{t_\mathrm{f}}, \ j \in I_\mathrm{fixed}, \tag{1c}$$

with (1b) modeling the reaction kinetics and (1c) the fixation of the RPVs (parameterization of the reduced model) at time $t = t_\mathrm{f}$. There are plenty of different approaches concerning a choice of a criterion $\Phi(z) = 0$ that (approximately) eliminates the fast modes of the system to obtain a POI (point of interest) on the SIM representing the reduced system. Since all methods share the same objective, there should be basic concepts underlying, combining, and unifying different approaches.

A. Derivative of the State Vector

One of those concepts is the derivative-of-the-state-vector-concept where time derivatives of the state vector are used, i.e. $\Phi(z)$ containing terms of type $\partial_t^m z(t)$. Model reduction methods exploiting this concept are e.g. the zero–derivative principle (ZDP) [4], the flow curvature method (FCM) [5], the intrinsic low dimensional manifold (ILDM) [12], and the stretching-based diagnostics [1].

B. Boundary Value Problem

A second fundamental concept for model reduction in dissipative kinetic systems with spectral gap is the boundary-value-concept which exploits the property of attractivity of SIMs. Provided that a SIM is globally attractive, every trajectory approaches it on infinite time horizon. In dissipative systems assuming $d\left(z(t_0), \mathrm{SIM}\right) > d\left(z(t_\mathrm{f}), \mathrm{SIM}\right)$ with $t_0 < t_\mathrm{f}$, where $d(\cdot,\cdot)$ is the (euclidian) distance function, and $z(t_\mathrm{f}) = z\left(t_\mathrm{f} - t_0, z(t_0)\right)$ (i.e. the solution of the initial value problem $\partial_t z(t) = S\left(z(t)\right), \ z(t_0) = z^{t_0}$ evaluated after a time period of $t_\mathrm{f} - t_0$), the POI identifies a SIM exactly for $t_\mathrm{f} - t_0 \to \infty$ and $d\left(z(t_0), \mathrm{SIM}\right) = c \in \mathbb{R}$ because of $d\left(z(t_\mathrm{f}), \mathrm{SIM}\right) = 0$. Having this in mind, the following general formulation of a boundary value problem for SIM computation/approximation is valid

$$\partial_t z(t) = S\left(z(t)\right), \ t \in [t_0, t_\mathrm{f}] \tag{2a}$$
$$z_j(t_\mathrm{f}) = z_j^{t_\mathrm{f}}, \quad j \in I_\mathrm{fixed} \tag{2b}$$
$$z_j(t_0) = K_j, \quad j \notin I_\mathrm{fixed} \tag{2c}$$

with $t_0 < t_\mathrm{f}$ in the *reverse mode*. Representatives of this concept are the saddle point method [2], [3], the invariant constrained equilibrium edge preimage curves (ICE-PIC) approach [13], and the reverse mode formulation of the trajectory-based optimization approach [9].

C. Two Concepts – One Approach

A specific example of a generalized formulation including both of these two conceptual ideas [11] is the following variational boundary value problem on a time horizon $[t_0, t_\mathrm{f}]$:

$$\min_{z(t)} \|\partial_t^m z(t)\|_2^2 \Big|_{t=t_0} \tag{3a}$$

subject to

$$\partial_t z(t) = S\left(z(t)\right), \;\; t \in [t_0, t_\mathrm{f}] \tag{3b}$$

$$z_j(t_\mathrm{f}) = z_j^{t_\mathrm{f}}, \;\; j \in I_\mathrm{fixed}. \tag{3c}$$

For realistic chemical kinetic models, the ODE model is defined only in a physically feasible region, a polyhedron in configuration space or a manifold, respectively, determined by additional constraints (e.g. species positivity, elemental mass conservation, possibly isenthalpic or other thermodynamic conditions) entering the optimization problem such that t_0 cannot be chosen arbitrarily small. Thus, for an accurate SIM approximation, the focus is on two issues in this context [11]:

- choosing m as large as practically possible (numerical computation of m-th order derivatives required),
- choosing t_0 as small as possible (considering the physically feasible domain).

This formulation relates our variational viewpoint [9] with the ZDP [4]. The original argument for the formulation of a trajectory-based variational problem for SIM computation was the following [6]: If a SIM exists, there should be some intrinsic property distinguishing trajectories on the SIM from others. The hope is to be able to find a criterion which formulates this differential property mathematically.

III. Variational Principle

In the light of a constrained variational boundary value problem formulation of SIM point computation [6], [7], [8], [9], necessary optimality conditions can be found using the first variation of the Lagrangian (or corresponding conditions in a Hamiltonian context) [11]. A boundary optimal control viewpoint can be taken and allows to relate SIM computation/approximation to (partial) integrability of dynamical systems and conservation properties which in turn are related to symmetry properties of the Lagrangian via Noether's theorem. The implications of these ideas will be discussed.

A. Symmetry and Criterion for SIM Computation

An exact criterion Φ for SIM point computation can be interpreted in the context of symmetry issues on an abstract level: The result of a species reconstruction technique for given RPVs (fixed number of variables and SIM dimension) parameterizing the SIM is a point in full state space – the POI. The SIM regarded as an intrinsic analytic object in state space should be coordinate independent, e.g. for any other choice (same total number) of RPVs the computed POI should coincide with the previous one. Thus, a necessary condition for an exact criterion characterizing the SIM is to yield POI results invariant under permutation of progress variables.

Reasoning on an error estimate quantifying in some sense the approximation property of SIM trajectories in relation to full state space trajectories might offer another viewpoint. Arguments by analogy from statistical mechanics on the relation of the dynamics of a macroscopic system state and its state variables (RPVs) to the consistent microscopic state (full composition) are discussed.

B. Composition Space–Time–Manifolds and Curvature

The composition space of the kinetic model equation can be extended by a time-axis allowing to regard the whole family of feasible solution trajectories as a smooth composition space-time manifold. We argue that a SIM might be characterized or at least approximated by an extremum principle based on differential geometric properties of this manifold. We point out relations to the geodesic structure of space-time in the theory of general relativity and discuss potential roles of curvature properties for SIM characterization.

IV. Application to Combustion Models

The algorithmic framework of numerical optimization for the solution of a variational formulation of the SIM computation problem offers high potential for efficient, robust and even real-time in situ computation of SIM points [10]. We demonstrate how sensitivity analysis based on the system of necessary optimality conditions of parametric optimization problems yields, along with the SIM points, a vector basis of the manifold's tangent space which can be exploited for an efficient embedding strategy for high-speed SIM computation. This is exemplarily demonstrated for a combustion model.

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