A Boundary Value View on the Reverse Trajectory-Based Optimization Approach for Kinetic Model Reduction

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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 is achieved via computation of slow manifolds which can be identified in these reaction systems. We discuss basic analytical components of model reduction by means of a linear test model and present a boundary value problem bundling ideas of many model reduction approaches.**

I. Introduction

Chemically reacting flows comprise an interplay between convective and diffusive species transport and chemical reaction processes involving a large number of chemical species and reactions. Together with the stiffness of the kinetic model equation with time scales ranging from nanoseconds to seconds, simulation of chemically reacting flows (for instance in combustion processes) is often nearly impossible in reasonable time. This calls for complexity reduction and multi-scale approaches.

Most of those model and complexity reduction techniques exploit the time scale separation of the model solution into fast and slow modes by approximating the large time scale system dynamics via eliminating the fast relaxing modes by enslaving them to the slow ones. This results in invariant manifolds of slow motion (SIMs) possessing the property of attracting system solution trajectories. The process of mapping a subset of the chemical species of the full model onto the full species composition by determining a point on a SIM is provided by an implicitly defined function. This *species reconstruction technique* is used by many model reduction approaches for SIM identification.

In this talk we discuss basic analytical issues of model reduction by means of a linear test model and present, why a (reverse) trajectory-based optimization approach suggested by Lebiedz [3] identifies SIMs exactly for an infinite time horizon [7] yielding the formulation of a boundary value problem.

II. Linear Test Model: Analytical Treatment

For simplicity we consider a two-dimensional linear ODE test model, representing chemical combustion model equation:

$$\partial_t z_1(t) = \left(-1 - \frac{\gamma}{2}\right) z_1(t) + \frac{\gamma}{2} z_2(t) \tag{1a}$$

$$\partial_t z_2(t) = \frac{\gamma}{2} z_1(t) + \left(-1 - \frac{\gamma}{2}\right) z_2(t), \quad \gamma > 0, \tag{1b}$$

with $\gamma \in \mathbb{R}$, $t \in \mathbb{R}$, $z_1, z_2 \in C^\infty(\mathbb{R}, \mathbb{R})$, and analytical solution

$$z_1(t) = c_1 \mathrm{e}^{-t} + c_2 \mathrm{e}^{(-1-\gamma)t} \tag{2a}$$

$$z_2(t) = c_1 \mathrm{e}^{-t} - c_2 \mathrm{e}^{(-1-\gamma)t}, \quad c_1, c_2 \in \mathbb{R} \tag{2b}$$

with c_i, $i = 1, 2$ being integration constants, to be determined by setting initial values. Due to the availability of explicit formula for the SIM, this model is well suited for analytical treatment. This formula is achieved by eliminating the fast modes (here implying setting c_2 equal to zero) yielding $z_1 \equiv z_2$ being the SIM. Subsituting this into (1) results in the following reduced model equation:

$$z_1(t) = z_2(t) \tag{3a}$$

$$\partial_t z_2(t) = -z_2(t) \tag{3b}$$

with analytical solution $z_1(t) = z_2(t) = c_1 \mathrm{e}^{-t}$ being equivalent to the solution of the full model (2) without fast modes ($c_2 = 0$).

Finding an additional criterion that automatically eliminates the fast modes without knowing the analytical solution of the underlying ODE model equations is the main challenge of model reduction approaches.

III. Slow Manifold Computation

A. Boundary Value Problem

In dissipative ODE systems where it holds that

$$d\left(z(t_0), \mathrm{SIM}\right) > d\left(z(t_*), \mathrm{SIM}\right) \tag{4}$$

with $t_0 < t_*$, $d(\cdot,\cdot) \in C^\infty(\mathbb{R}^n \times \mathbb{R}^n, \mathbb{R})$ being the distance function, and $z(t_*)$ meaning $z(t_*) = z\left(t_* - t_0, z(t_0)\right)$ (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 $t_* - t_0$), the point of interest (POI) $z(t_*)$ identifies a SIM exactly for $t_* - t_0 = \infty$ and $d\left(z(t_0), \mathrm{SIM}\right) \in \mathbb{R}$:

$$d\left(z(t_*), \mathrm{SIM}\right) = 0. \tag{5}$$

Having this in mind, the following general formulation of a boundary value problem for SIM computation is presented:

$$\partial_t z(t) = S\left(z(t)\right) \tag{6a}$$

$$z_j(t_*) = z_j^{t_*},\ \ j \in I_{\text{fixed}},\ \ t_* \in \mathbb{R} \tag{6b}$$

$$z_j(t_0) = K_j,\ \ j \notin I_{\text{fixed}},\ \ K_j = \text{const.}\ \wedge\ |K_j| \neq \infty\ \forall j \notin I_{\text{fixed}} \tag{6c}$$

with $t_0 < t_*$ in the reverse mode formulation [7], [8]. Here, (6a) describes the system dynamics, (6b) the fixation of those variables that parameterize the SIM at time $t = t_*$, and I_{fixed} denotes the index set containing those *reaction progress variables*. For globally attractive systems the choice of K is without significance to achieve $\lim_{t_0 \to -\infty} z(t_*) \in$ SIM, whereas in realistic chemical processes the choice of K plays a significant role caused by additional physical constraints restricting the area where the ODE model is defined and thus, t_0 can only be chosen as small as possible. This idea of using a boundary value method for slow manifold computation is also found in [2], [9], [10] for example. Exact SIM identification by using this reverse boundary value problem with an infinite time horizon is confirmed by analytical and numerical tests applying the linear model (1) (see [8]).

B. Trajectory-Based Optimization Approach and Zero-Derivative Principle

For a 'good choice' of K we use the derivative idea from the Zero-Derivative Principle (ZDP) [1], [11] (POI is closer to SIM with higher derivatives) and relate it to the trajectory-based optimization approach [3], [4], [5], [6], [7] leading to the following formulation of a model reduction technique combining both the boundary value idea from above and the derivative idea of the ZDP:

$$\min_{z(t)} \|\partial_t^m z(t)\|_2^2\Big|_{t=t_0}, \quad m \in \mathbb{N} \tag{7a}$$

subject to

$$\partial_t z(t) = S\left(z(t)\right) \tag{7b}$$

$$0 = g\left(z(t_*)\right), \quad t_* \in \mathbb{R} \tag{7c}$$

$$z_j(t_*) = z_j^{t_*}, \quad j \in I_{\text{fixed}} \tag{7d}$$

with $g \in C^\infty\left(\mathbb{R}^n, \mathbb{R}^b\right)$ containing possible additional constraints (for instance chemical element mass conservation relations) and can be omitted for the linear test model above. In this formulation K improves with higher m yielding

$$\lim_{m \to \infty} z(t_*) \in \text{SIM} \tag{8a}$$

$$\lim_{t_0 \to -\infty} z(t_*) \in \text{SIM}. \tag{8b}$$

Both analytical and numerical computations confirm these results.

In numerical implementations for realistic combustion processes difficulties arise from choosing $m > 2$. The kinetic ODE model is only defined on a polyhedron in phase space based on additional constraints entering the optimization problem such that t_0 cannot get arbitrarily small. Thus, for a good SIM approximation in realistic models two issues have to be addressed:

- choosing m as large as possible.
- choosing t_0 as small as possible.

C. How to Treat Constraints in Realistic Kinetic Models

Since the POI improves with smaller t_0, the aim is a minimal feasible choice of t_0. We address this issue via analytical treatment for the linear model (1).

Solving (7) with (1) analytically provides analytical formula for the integration constants from (2) $\hat{c}_1$ and $\hat{c}_2$ dependent on t_0 which are substituted into $z_1 = z_1(\hat{c}_1, \hat{c}_2)$ and $z_2 = z_2(\hat{c}_1, \hat{c}_2)$ for solving the following optimization problem yielding the minimal t_0 that is feasible

$$\min t_0 \tag{9a}$$

subject to

$$z_1(\hat{c}_1, \hat{c}_2) \geq 0 \tag{9b}$$

$$z_2(\hat{c}_1, \hat{c}_2) \geq 0 \tag{9c}$$

$$z_1(\hat{c}_1, \hat{c}_2) \leq n_1 z_2(\hat{c}_1, \hat{c}_2) + b_1 \tag{9d}$$

$$z_1(\hat{c}_1, \hat{c}_2) \leq n_2 z_2(\hat{c}_1, \hat{c}_2) + b_2 \tag{9e}$$

with (9b)–(9e) being the additional constraints entering the model reduction above as function g. Solving (9) with different choices of the constants results in a minimal feasible choice of t_0.

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