CONSIDERING SLOW MANIFOLD BASED MODEL REDUCTION FOR MULTISCALE CHEMICAL OPTIMAL CONTROL PROBLEMS

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ABSTRACT

Finite-dimensional dissipative dynamical systems with multiple time-scales are obtained when modeling chemical reaction kinetics with ordinary differential equations. Such stiff systems are computationally hard to solve and therefore, optimal control problems which contain chemical kinetic models as infinitesimal constraints are even more difficult to handle. Model reduction might offer an approach to improve numerical efficiency as well as avoid stiffness of such models. We show in this paper for benchmark problems how attracting manifold computation methods could be exploited to solve optimal control problems more efficiently while having in mind the ambitious long-term goal to apply them to real-time control problems in chemical kinetics.

Keywords Optimal Control · Model Order Reduction · Singular Perturbation Theory · Slow Invariant Manifold · Numerical Optimization

1 Introduction

Modeling chemical reaction mechanisms with ordinary differential equations (ODEs) yields highly-nonlinear systems with multiple time-scale dynamics. This makes them computationally hard to control online, e.g. with nonlinear model predictive control (NMPC). Thus, model reduction methods can be considered to tackle such problems.

A class of model reductions that can used in the context of multiple time-scale dynamics is the class of manifold-based model reduction methods (for an overview see e.g. Lebiedz and Unger[1]). Since the long time behavior of such systems is dominated by the slow components which are often stable, the system usually approaches low-dimensional manifolds in the phase space divided into slow and fast components, i.e. the slow invariant manifold is attracting.

It is still an open issue how these manifolds can be used to simplify and accelerate the computations of optimal control problems. First investigations towards this goal have been performed by Rehberg [2, 3]. In this paper, we show how (point-wise) online computation of such manifolds can be integrated into the multiple shooting based solution of optimal control problems in a reasonable and useful way. Two low-dimensional benchmark problems demonstrate the efficiency of this method.
1.1 Classification of Model Reduction Methods

Modern model order reduction methods commonly in use for optimal control, in particular in large-scale partial differential equation (PDE) applications, can roughly be divided into at least three categories: Krylov based methods, singular value decomposition (SVD) based methods and trajectory based methods. In particular, the latter is a nonlinear method, whereas the former two have originally been developed for large linear systems. We give a brief description of them and list some of their main characteristics, advantages as well as disadvantages.

**Krylov Based Methods** project systems onto Krylov subspaces. A widely used technique of this category is the moment matching method [4] which interpolates derivatives (moments) of the transfer function for linear, time-independent systems at certain points. Arnoldi- or Lanczos processes are used for the projection onto the Krylov subspaces and can be implemented efficiently. But there exists no global error bound.

**In SVD Based Methods** high-dimensional, high-rank matrices $M$ are approximated by matrices $M_k$ of lower rank $k$ using singular value decomposition. Furthermore, these rank $k$ approximations are optimal in unitarily invariant norms and for the Euclidean norm. The replacement of the original matrix and its approximation is determined by the $(k+1)$-th largest singular value. A very popular SVD based method is balanced truncation [5]. It balances linear, time-independent systems such that their controllability and observability Gramians become diagonal and equal. Negligible states are truncated such that asymptotic stability can be preserved. A priori error bounds are computable.

For nonlinear and time-dependent systems the probably most successful method is proper orthogonal decomposition (POD). The key idea of POD is to compute samples of the trajectory - so called snapshots - and use SVD in order to construct a basis of a subspace of the snapshot space. However, as described in Chaturantabut and Sorensen [6], the computational complexity of the reduced model is almost as high as for the original model, if the system is very nonlinear. To overcome this difficulty, for example Empirical Interpolation Methods [6], [7] are used. For a more detailed overview of the SVD based methods and the Krylov based methods see Antoulas and Sorensen [8] or Benner, Sachs, and Volkwein [9].

**Trajectory Based Methods** are totally different in nature, they are fully nonlinear, aimed at a replacement of the full (usually linear) state space by a (nonlinear) manifold of lower dimension. They are based on time scale separation which arises for example in models of chemical kinetics. The state space is not projected onto a linear or affine subspace but onto a lower dimensional manifold. So the nonlinearity of the problem is somehow encoded in the manifold. Maas and Pope [10] introduced the intrinsic low-dimensional manifolds (ILDM) method which uses the structure of a spectral decomposition of the Jacobian of the vector field. Decoupling slow and fast submatrices yields a good approximation of the slow invariant manifold (SIM). The reduced model also has the benefit of less stiff dynamics. A drawback of this method and manifold-based approaches in general is that there are no reliable a priori error bounds.

In this paper, we restrict ourselves to a subclass of trajectory based methods based on some of the authors’ previous work. Our model order reduction approach [11] [12] [13] [14] [15] [16] is based on either a nonlinear root finding problem or a equation of a variational principle for approximation of trajectories on slow (attracting) invariant manifolds.

Both POD and trajectory based methods exploit a contraction property of the dynamical systems for the construction subspaces. We choose a trajectory based method for optimal control in the context of chemical reactions because of the high nonlinearity and stiffness that come with chemical dynamics.

The paper is organized as follows. A brief introduction to manifold-based model reduction is given in Section 2 and two successful numerical model reduction methods are presented. A new approach to combine manifold-based calculation of slow manifolds and optimal control problems is introduced. Numerical methods for the solution of optimal control problems can be found in Section 3, results are in Section 4 and a conclusion follows in Section 5.

2 Model Reduction Methods for Multi-Scale Systems

Let a general system be given by

$$\dot{z}(t) = f (z(t)) \quad \forall t \in [0, T], \quad (1)$$

where $f \in C^r(\mathbb{R}^n, \mathbb{R}^n)$ for a number $r \in \mathbb{N} \cup \{\infty\}$, i.e. $f$ is a $r$-times continuously differentiable function, that maps from $\mathbb{R}^n$ to $\mathbb{R}^n$. In the following we assume that system (1) has multiple time-scales, i.e. the eigenvalues $\lambda_1 \leq \ldots \leq \lambda_n$ of the Jacobian of $f$ at the equilibrium (a root of $f$) are clustered in the sense that there exists a $1 \leq k \leq n - 1$ such that $\lambda_1 \leq \ldots \leq \lambda_k \ll \lambda_{k+1} \leq \ldots \leq \lambda_n$. In the phase space of such systems often there exists a manifold which is invariant under the flow of the dynamics (1) and that is characterized by a fast bundling of trajectories onto this manifold. For a given initial value, the correspond-
The first approach suggested by Lebiedz and Unger is motivated mainly by the fol-
with the flow.

Theorem 1 is the theoretical basis and motivation of manifold-based model reduction for singularly perturbed systems.

In the following, \( (z_s(t), z_f(t)) \) will often be abbreviated by \( z(t) \) and correspondingly \( (f_s, f_f) \) will be abbreviated by \( f \).

In the following, we will shortly present numerical methods that are able to calculate points of the SIM. The error \( e(t) := \| z_f(t) - h_{app}(z_s(t)) \| = \| h_{\varepsilon}(z_s(t)) - h_{app}(z_s(t)) \| \) should be as small as possible, however in general we have no error estimates. In case of stable systems this usually does not give rise to severe problems in applications since the error decreases exponentially with time while the dynamical system state evolves with the flow.

**2.1 Methods for the Approximate Calculation of the SIM**

In the following we will shortly present numerical methods that are able to calculate points of the SIM approximately and that proved to be successful in slow manifold computation, i.e. approximations for the function \( h_{\varepsilon}(\cdot) \). These methods represent functions \( h_{app} : \mathbb{R}^{n_s} \rightarrow \mathbb{R}^{n_f} \) such that the point \( (z^*_s, h_{app}(z^*_s)) \) is located in a close neighborhood of the SIM. The error \( e(t) := \| z_f(t) - h_{app}(z_s(t)) \| = \| h_{\varepsilon}(z_s(t)) - h_{app}(z_s(t)) \| \) should be as small as possible, however in general we have no error estimates. In case of stable systems this usually does not give rise to severe problems in applications since the error decreases exponentially with time while the dynamical system state evolves with the flow.

**Approach Lebiedz/Unger** The first approach suggested by Lebiedz and Unger is motivated mainly by the fol-
with the flow.

Theorem 1 is the theoretical basis and motivation of manifold-based model reduction for singularly perturbed systems. Fenichel [17] showed the existence of the SIM in the form of Theorem [11, 12, 13, 14, 15, 16].

**Remark 2.** As the fast variables \( z_f \) can be reconstructed out of the slow variables \( z_s \), if the manifold mapping \( h_{\varepsilon} \) is known, the slow variables are the so called reaction progress variables (RPVs).

In the following, \( (z_s(t), z_f(t)) \) will often be abbreviated by \( z(t) \) and correspondingly \( (f_s, f_f) \) will be abbreviated by \( f \).

Theorem [1] is the theoretical basis and motivation of manifold-based model reduction for singularly perturbed systems since system (2) can be reduced to

\[ z_s(t) = f_s(z_s(t), h_{\varepsilon}(z_s(t)); \varepsilon) \quad \forall t \in [0, T]. \tag{3} \]

This reduced system (3) is of smaller dimension than (2) and our calculations in Section [4] show that it is less stiff because fast time scales have been eliminated. Especially, the second property is numerically important as we will see in Section [4]. However, Theorem [1] does not provide any efficient method for the calculation of \( h_{\varepsilon} \).

**minimize**  
\( z(\cdot) = (z_s(\cdot), z_f(\cdot)) \)  
\( \| \dot{z}(t_0) \|_2^2 \)  

**such that**  
\( \dot{z}(t) = f(z(t)) \),  
\( 0 \leq c(z(t)) \),  
\( z^*_s = z_s(t_1) \).  

(4a)  
(4b)  
(4c)  
(4d)
The choice of \( t \)
The Zero Derivative Principle (ZDP) \cite{19} The idea for the Zero Derivative Principle is to eliminate fast dynamical modes by zeroing higher-order derivatives of the vector field. For a given slow components vector \( z_s^* \), the ZDP identifies a point \( z_f^* \) in terms of a root finding problem:

\[
\frac{d^m z_f}{d t^m} = 0 \quad \text{for a given } m \in \mathbb{N}.
\]  

For example, if \( m = 2 \) the ZDP equation \eqref{ZDP} can be rewritten to

\[
\frac{d^2 z_f}{d t^2} = \frac{d}{d t} f_f(z_s^*, z_f^*; \varepsilon) = \frac{\partial f_f(z_s^*, z_f^*; \varepsilon)}{\partial z_f} \cdot f_f(z_s^*, z_f^*; \varepsilon)
\]

using the chain rule and is thus very similar to \eqref{local} in the local approach. Further, \eqref{local} can be seen as a root finding problem of the function

\[
\psi(z_f) = \frac{\partial f_f(z_s^*, z_f^*; \varepsilon)}{\partial z_f} \cdot f_f(z_s^*, z_f^*; \varepsilon).
\]

Zagaris et al. \cite{20} show that the difference between the SIM (given by Fenichel’s definition in terms of an \( \varepsilon \)-series) and \( h_{\text{app}} \) (here: root of \( \psi \)) given by the ZDP is \( e(t) = O(\varepsilon^m) \).

The ZDP was generalized by Benoit, Brøns, Desroches and Krupa \cite{21}. So, the SIM can also be approximated by setting the time-derivatives of the slow components to zero. If the derivative of the \( i \)-th component of \( f_s \) w.r.t. \( z_s \) for a given point \((z_s^*, z_f^*)\) is regular then the equation \eqref{generalized ZDP}

\[
\frac{d^m z_s}{d t^m} = 0 \quad \text{for a given } m \in \mathbb{N}
\]

gives an approximation of the SIM up to order \( O(\varepsilon^{m-1}) = e(t) \).

Since the SIM is intrinsically characterized by the dynamics, it should be possible to calculate the SIM for an arbitrary choice of the slow variables (thus, the SIM should be represented in coordinate-independent form). Therefore, a reasonable numerical method should also be invariant under such a choice of “slow variable parametrization”. The generalized ZDP shows that this is possible in principle. However, the generalized ZDP method is strictly speaking not coordinate-free, because an explicit choice of slow variables has to be made and the numerical result slightly depends on this choice.

It should be mentioned that the ZDP method is local, i.e. only in a neighborhood of \((z_s^*, z_f^*, 0)\) the ZDP method

\[
\frac{d^m z_f}{d t^m} = 0
\]

yields an error approximation \( e(t) = O(\varepsilon^m) \). A priori it is not clear how large this neighborhood is. So, in practice one has to carefully check and evaluate the numerical solution.

\[2.2\] Slow Manifold Based Optimal Control

Consider ODE constrained optimal control problems (OCP) in the following form:

\[
\begin{align*}
\text{minimize} & \quad L(z_s(t), z_f(t), u(t)) \, dt \\
\text{such that} & \quad \dot{z}_s(t) = f_s(z_s(t), z_f(t), u(t); \varepsilon), \quad \text{for } t \in [0, T], \\
& \quad \varepsilon \dot{z}_f(t) = f_f(z_s(t), z_f(t), u(t); \varepsilon), \quad \text{for } t \in [0, T], \\
& \quad 0 \leq c(z(t)), \\
& \quad z_s(0) = z_s(0), \\
& \quad z_f(0) = z_f(0).
\end{align*}
\]
where \( z_s(t) \in \mathbb{R}^{n_s}, z_f(t) \in \mathbb{R}^{n_f} \) with control \( u(t) \in \mathbb{R}^{n_u} \), for \( t \in [0, T] \). In the following, we will refer to (8) as the original or full problem. We will use it as reference problem for the comparisons of Section 4.

In realistic chemical reaction mechanisms this full OCP often cannot be solved in real-time, because either the total number of optimization variables or the stiffness of ODE (2) prevents numerical algorithms from calculating local optima efficiently.

A possibility to reduce its dimension is to insert the manifold mapping \( h \), where

\[
\psi(z_s, z_f, u) := \begin{cases} 
  z_s & \text{for } t \in [0, T], \\
  z_f - h_{\text{app}}(z_s, u) & \text{otherwise},
\end{cases}
\]

where again \( h_{\varepsilon}(z_s) \) can be numerically approximated by \( h_{\text{app}} \) resulting from the Lebiedz/Unger or the ZDP approach.

Note that the controls \( u(t) \) are regarded as “slow” variables, because of several reasons. In chemical reactions the fast time scale is often too fast for precise control of input species. In the next section we discretize \( u(t) \) and the other states in time and use piecewise constant values to approximate \( u(t) \). This prevents the optimal control from chattering with a huge number of switches and constant values are directly related to slow variables.

The dynamics of (9b) are less stiff than those of (8) and (9) has just \( n_s + n_u \) instead of \( n_s + n_f + n_u \) optimization variables. Numerically however, \( h_{\varepsilon}(\cdot) \) in problem (9) will be approximated by a root finding respectively optimization problem, which has to be solved in each iteration of any algorithm for optimization problem (9).

### A New Approach for Efficiently Solving Manifold-Based OCPs

The new approach we propose is based on the idea of lifting, as first presented in Albersmeyer and Diehl[22]. To prevent numerical solvers from calculating \( h_{\varepsilon}(z_s, u) \) respectively \( h_{\text{app}}(z_s, u) \) exactly in each iteration of (9) the equation \( z_f = h_{\varepsilon}(z_s, u) \) is handled as a constraint of the OCP. The numerical solution has to satisfy this equation, but not other iterates, which cuts computational costs. In comparison with the original OCP (8), the dynamics (8b) and (8c) are replaced by the following differential algebraic equation (DAE) (10):

\[
\begin{align*}
\dot{z}_s &= f_s(z_s, z_f, u; \varepsilon) \\
0 &= z_f - h_{\varepsilon}(z_s, u).
\end{align*}
\]

Using the methods of Lebiedz/Unger or ZDP for the approximation of \( h_{\varepsilon} \) (both can be written as root finding problems \( \psi = 0 \)), we get the following OCP (11):

\[
\begin{align*}
\text{minimize} & \quad \int_0^T L(z_s, z_f, u) \, dt \\
\text{such that} & \quad \dot{z}_s = f_s(z_s, z_f, u; \varepsilon), \\
& \quad 0 = z_f - h_{\varepsilon}(z_s, u), \\
& \quad z_s(0) = z_s(0), \\
& \quad z_f(0) = z_f(0).
\end{align*}
\]

In the following, we will refer to (9) as the reduced OCP and to (11) as the lifted OCP. It has the same number of optimization variables like the full OCP (8) and its dynamics (11b) are less stiff such that the usage of an explicit integrator is often justified.

### 3 Numerical Solution

The choice of numerical solution method for OCPs (8), (9), (11) is an important decision to make in order to target real-time applications.

We will solve said OCPs with a direct approach. More precisely, we choose a multiple shooting discretization [23], which has been proven to work well and efficiently in practice [24]. We take \( N \) shooting intervals, on which we
simulate the slow dynamics using an explicit Runge-Kutta integrator of order 4, where we take 1 integration step per shooting interval. Note that the explicit integration method is only suited for the reduced and lifted problem formulations. For the full problem, we use an implicit integration scheme, namely a stiffly accurate Radau II-A method. For all methods discussed, we model the controls as piecewise constant over one shooting interval.

We noted before that the new efficient method for solving manifold-based OCPs is compatible with either the Lebiedz/Unger approach or with the ZDP. In the latter case, we are free to pick any \( m \), such that the \( m \)-th time derivative should be equal to zero (see Section 2.1). We chose \( m = 2 \), as it is a good trade-off between accuracy (recall that the error is \( \mathcal{O}(e^m) \)) and computational cost of forming the derivatives.

Carrying out the discretization yields a finite-dimensional nonlinear programming problem (NLP), which we then solve with a Newton-type optimization method. More specifically, we use the interior point solver IPOPT [25], which is a powerful algorithmic differentiation routines for the higher-order derivatives of the functions present in the OCP, such that we are able to use exact Hessians in our solution method.

We remark that different choices for discretization of the problem exist. The multiple shooting method is chosen, because it widely spread for optimal control problems with PDE and ODE constraints. Its advantages are numerical stability (e.g., in contrast with the single shooting) and the usage of a moderate number of optimization variables. Therefore, it is often used for high-dimensional optimal control problems.

For readers that are familiar with CasADi it should be mentioned that in the implementation of the different approaches SX variables are used whenever it is possible and MX variables are only used for implicit integrators. Symbolic SX expressions are typically longer, but faster to evaluate in comparison with MX expressions. However, MX expressions are more flexible with a larger range of applications, e.g., for root-finding problems based on Newton’s method.

4 Results

For all numerical experiments an Ubuntu 18.04 machine with an Intel® Core™ i7-2600 (8 cores with 3.40 GHz) CPU and 16 GB RAM is used. The software version R2018a of MATLAB and version 3.4.4 of CasADi are installed.

The following examples serve as first benchmark problems and do not have a deeper meaning or specific aim in mind. The objective functions are artificial.

4.1 Enzyme Example

A simple chemical reaction mechanism with enzymes is given by the Michaelis-Menten-Henri mechanism (cf. example 11.2.4 in Kuehn [18])

\[
S + E \rightleftharpoons C \rightarrow P + E,
\]

where \( S \) is a substrate, \( E \) is an enzyme, \( C \) the corresponding substrate-enzyme-complex and \( P \) a product. Simplifying the ODE [27] which underlies (12) and introducing an artificial objective function yields optimal control problem [13].

\[
\begin{align*}
\text{minimize} & \quad \int_0^5 -50z_f(t) + u^2(t) \, dt \\
\text{such that} & \quad z_s(t) = -z_s(t) + (z_s(t) + 0.5)z_f(t) + u(t), \quad \text{for } t \in [0, 5], \\
& \quad \varepsilon z_f(t) = z_s(t) - (z_s(t) + 1)z_f(t), \quad \text{for } t \in [0, 5], \\
& \quad 1 = z_s(0),
\end{align*}
\]

where \( z(\cdot) = (z_s(\cdot), z_f(\cdot)) \in \mathbb{R}_+ \times \mathbb{R}_+ \) and control \( u(t) \in [0, 10] \) represents the possibility to add some substrate (corresponds to variable \( z_s \)) to the system.

The numerical results for this example discretized in \( N = 40 \) subintervals and with \( \varepsilon = 10^{-6} \) can be seen in Figures 11 [28] and 4 [29]. The solutions of the original system (8) and lifted system (11) are almost equal. To be more precise, it holds

\[
\max \left\{ \|z_s^{\text{orig}} - z_s^{\text{app}}\|_\infty, \|z_f^{\text{orig}} - z_f^{\text{app}}\|_\infty, \|u^{\text{orig}} - u^{\text{app}}\|_\infty \right\} = \|z_s^{\text{orig}} - z_s^{\text{app}}\|_\infty \approx 0.047,
\]

\[\varepsilon \in [1, 3] \quad \text{and} \quad \varepsilon \leq 10^{-5} \]

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which gives a relative error smaller than 1.16 % (except of the last control $u_N$ that is almost zero). The objective function values produce a relative error of 0.21 % (the objective function value is about -187.85). For brevity, we omit the numerical solution of the direct collocation method here. The errors between the multiple shooting and the collocation solution are comparable to the errors between the multiple shooting of the full OCP and the lifted OCP. Just the difference in the numerical values for $z_s$ is a little bit bigger. To sum up, there is no big difference in the quality of the solutions.

Figure 1: Numerical solution of (8) with multiple shooting.

Figure 2: Numerical solution of (11) using the ZDP with $m = 2$.

Figure 3: absolute error between full (8) and lifted solution (11).

Figure 4: relative error between full (8) and lifted solution (11).

However, there is a big difference in the runtimes which are listed in Table 1. Whereas the NLP resulting from the original system can be solved with CasADi/Ipopt in 0.1688 seconds, our proposed approach using ZDP of order $m = 2$ only needs 0.0224 seconds. This gives a significant speed up of factor 7.5. The order reduced OCP (9) takes 0.5272 seconds. It has the smallest number of optimization variables, but the nested root finding problem for $h_\varepsilon(\cdot)$ in each interval causes this longer runtime. As already mentioned in Rehberg [2], the order reduced OCP (9) does not need to improve the runtime, although less optimization variables are present.

For other values of $\varepsilon \in (0, 0.1]$ and the choice of $z_s(0)$ almost the same runtimes are obtained for both the full problem and the lifted problem.

4.2 CSTR Example

Inspired by an example of Cvejn [23], we consider a small continuous stirred-tank reactor (CSTR) in which the chemical reactions

$$A \overset{k_1}{\underset{k^-_1}{\rightleftharpoons}} B \rightarrow C \overset{k_2}{\rightarrow} D$$

take place for given reaction rates $k_1, k^-_1, k_2$ and $\varepsilon$. For simplicity, we assume that the tank is perfectly mixed and the reaction is isothermic. Figure 5 illustrates the CSTR. Input for the reaction is only species $A$ with a given (constant) concentration $c_{A_0}$. This input can be controlled via a feed $q_A \in [0, q_{A_{max}}]$. Output of the reactor is a mixture of species $A, B, C$ and $D$ and can also be controlled with the outlet $q \in [0, q_{max}]$. A possible scenario is that the number of moles
of species $B$ should be maximized in the output of the CSTR. Since the volume of the tank reactor is bounded, this leads to an optimal control problem with constraints (see \eqref{eq:14}). For brevity, we omit the arguments of the functions in the ODE part of the OCP (i.e. the dependency on $t$).

\begin{align*}
\text{minimize} & \quad \int_0^{500} -0.1 q \cdot c_B + q_A^2 + q_A^2 \, dt \\
\text{such that} & \quad c_A' = -k_1 c_A + k_1 c_B + \frac{q_A}{V} (c_{A_0} - c_A), \\
& \quad c_B' = k_1 c_A - (k_1 + \varepsilon) c_B - \frac{q_A}{V} c_B, \\
& \quad c_C' = \varepsilon c_B - k_2 c_C - \frac{q_A}{V} c_C, \\
& \quad c_D' = k_2 c_C - \frac{q_A}{V} c_D, \\
& \quad \dot{V} = q_A - q, \\
& \quad c^* = c(0), \\
& \quad V^* = V(0) = V(500),
\end{align*}

where $c(t) = (c_A(t), c_B(t), c_C(t), c_D(t))^T$ and $c^* = (c^*_A, c^*_B, c^*_C, c^*_D)^T$. The values of the constants in OCP \eqref{eq:14} can be taken from Table \ref{tab:2}.

Note that the ODE of this OCP is not in singularly perturbed form. However, the idea of lifting in combination with the ZDP method is still applicable, because its dynamics are given by a multi-scale ODE. The choice of reaction progress variables is not obvious and has combinatorial complexity. We choose $B, D$ and the volume $V$ mainly motivated by the reaction rates.

For $N = 140$ intervals IPOPT converges to a point of local infeasibility for the nonlinear program resulting from the lifted OCP using multiple shooting and ZDP of order 2. Without the constraint $c_A(0) = c_A^*$, it converges to the solution depicted in Figures \ref{fig:6}, \ref{fig:7}, \ref{fig:8}, \ref{fig:9}, and \ref{fig:10}. For the plots of the lifted OCP, we took the optimal controls of the numerical solution and integrated the other states forward in time with an implicit Radau II-A integrator.
The solutions of the original system (8) via multiple shooting and the lifted system (11) (without forward integration) are, in contrast to the enzyme example, not almost equal. It holds

\[
\max \left\{ ||c_{\text{orig}} - c_{\text{app}}||_{\infty}, ||q_{\text{orig}} - q_{\text{app}}||_{\infty}, ||q'_{\text{orig}} - q'_{\text{app}}||_{\infty} \right\} = ||c_{\text{orig}} - c_{\text{app}}||_{\infty} \approx 0.049.
\]

This can also be observed in Figures 6 and 7. Variable \(c_B\) in the lifted OCP grows more rapidly at the beginning of the time interval. IPOPT has found two different optimal solutions (for two different nonlinear problems). The objective function values are \(-0.25667\) for the full system and \(-0.25679\) for the lifted system which yields an absolute difference of \(1.2 \cdot 10^{-4}\) and a relative difference of about \(0.047\%\).

Averaged runtimes for all methods mentioned above can be found in Table 3. Because of the slowness of the reduced OCP, we did not implement this approach for the CSTR example. The relations of the runtimes are comparable to those of the first example. For the lifted systems including the ZDP method of order \(m = 2\) a significant speed up of factor 38 in comparison with the full multiple shooting method is observed.

Depending on the number of intervals, the solution of the full system changes. For \(N = 4000\) intervals, the solution of the full OCP via multiple shooting (see Figures 12, 13, and 14) looks qualitatively more like the lifted solution for \(N = 140\) than like the solution of the full OCP. The objective function value is \(-0.2568167\). These facts point out the sensitivity of the problem as well as the benefits of the lifted OCP.

5 Conclusion

In this paper, we show by help of benchmark problems that it is possible to use slow manifold based model reduction techniques in order to solve optimal control problems (OCPs) with multiple time-scale dynamics based on multiple...
shooting faster but slightly less accurate. For this reason, the dynamics of the fast optimization variables are replaced by nonlinear equality conditions. The benefit of that approach is not visible at first sight since the system we get in this way is of the same order – so we cannot speak of model order reduction in proper meaning of the word. However, the remaining ODE part of the OCP is much less stiff. This allows us to use explicit integrating routines rather than implicit integrators to solve the ODE part numerically.

Numerical experiments have shown that this approach gives a speed-up of factor 7 to 38. Since the new approach differs from the original OCP, in general different solutions are expected. But, the corresponding objective function values differ just slightly.

A goal for future research is to improve the new approach in order to be able to solve OCPs with stiff chemical kinetic ODE constraints in real-time.
Figure 14: “full” volume $V$ of (8) solved by multiple shooting on $N = 4000$ intervals.

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### A Tables

Table 1: Runtimes in seconds, the number of variables and constraints for the underlying NLP of the enzyme example with \( N = 40 \).

| method                              | runtime | #variables | #constraints |
|-------------------------------------|---------|------------|--------------|
| full OCP (multiple Shooting)        | 0.1688  | 120        | 80           |
| reduced OCP (ZDP \( m = 2 \))      | 0.5272  | 80         | 40           |
| lifted OCP (Lebiedz/Unger)         | 0.0268  | 121        | 80           |
| lifted OCP (ZDP \( m = 2 \))      | 0.0224  | 121        | 80           |

Table 2: Constants for the CSTR example

| constant | description                                | value |
|----------|--------------------------------------------|-------|
| \( c_{A_{in}} \) | concentration of species \( A \) of inlet | 1     |
| \( k_1 \) | forward reaction rate constant of \( A \rightleftharpoons B \) | 100   |
| \( k^-_1 \) | backward reaction rate constant of \( A \rightleftharpoons B \) | 90    |
| \( k_2 \) | reaction rate constant of \( C \rightarrow D \) | 20    |
| \( \varepsilon \) | reaction rate constant of \( B \rightarrow C \) | \( 10^{-6} \) |
| \( q_{A_{max}} \) | maximum value for \( q_A \) in inlet | \( 10^{-3} \) |
| \( q_{max} \) | maximum value for \( q \) in outlet | \( 1.5 \cdot 10^{-3} \) |
| \( c_A^* \) | initial concentration of species \( A \) | \( 10^{-3} \) |
| \( c_B^* \) | initial concentration of species \( B \) | \( 10^{-3} \) |
| \( c_C^* \) | initial concentration of species \( C \) | 0     |
| \( c_D^* \) | initial concentration of species \( D \) | \( 10^{-8} \) |
| \( V^* \) | initial and final volume of tank reactor | \( 10^{-2} \) |

Table 3: Runtimes for the CSTR example in seconds for \( N = 140 \).

| method                              | runtime | #variables | #constraints |
|-------------------------------------|---------|------------|--------------|
| full OCP (multiple Shooting)        | 5.0817  | 979        | 700          |
| lifted OCP (Lebiedz/Unger)         | 0.2473  | 980        | 700          |
| lifted OCP (ZDP \( m = 2 \))      | 0.1311  | 980        | 700          |