Global Reduction Method for Chemical Kinetic Models

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Introduction

There has been significant progress over last years in hardware and software development. Novel powerful software packages simplify significantly not only the actual numerical simulation part (CHEMKIN, COSILAB etc.), but also the development stage of the mathematical model has become almost automatic. As a result large elementary reaction mechanisms have been designed to improve chemical reaction models for a better understanding of the governing processes. Furthermore, in order to increase efficiency and to advance the design of industrial, engineering and technological tools as well as biotechnology, structural molecular design etc. more sophisticated detailed models have to be developed, simulated and analyzed. This leads to an enormous growth of a system of governing differential equations in both dimension and complexity. Therefore, it is desirable to reduce models complexity without significant loss of the overall qualitative and quantitative properties by comparison with the original one. A large number of practical systems demonstrate essentially different time scales for different subsystems. This discrepancy in time scales leads to multi-scale nature of detailed mathematical models. We developed a robust and efficient global decomposition/reduction method for such multi scale models based on a coordinate free concept of singularly perturbed system of differential equations (so-called singularly perturbed vector fields).

Global Decomposition

Multi scale models with an explicit small parameters are the main subject of the theory of singularly perturbed system of differential equation (SPS). Using this well developed theory original models with an explicit small parameter can be decomposed and/or reduced to low dimensional models using the theory of fast and slow integral/invariant manifolds. The main obstacle with practical applications of the SPS theory is an implicit nature of a multi scale structure namely, for complex realistic models this structure is "hidden" in the original model. Sometimes (for comparatively simple models) such structure can be rearranged until explicit one, using physical or engineering knowledge about the processes under investigation. In the general case, the transition from the original system with the "hidden" multi scale structure to a system with an explicit representation of this structure is not evident. In good cases it requires a detailed analysis of the mathematical models properties and also a large amount of time (human resources) to find a particular decomposed form, which, in turn, can vary from one parametric region to another.

Thus an automatic procedure for model reduction is required, which is based on the assumption of a global multi-scales structure existence for an original system of governing equations. Under such assumption the only problem which has to be solved is the automatic transformation of the original system into the standard SPS form. In the case that such transformation is found the original model can be rewritten by an equivalent way

as a standard explicit singularly perturbed system that can be treated by a reasonable combination of numerical and analytical methods. From a purely mathematical point of view we are looking for a new coordinate system that permits an explicit representation of an original multi scale model as a system of differential equations with explicit small parameter (parameters).

As a theoretical background for a convenient algorithm we use a new concept of singularly perturbed vector fields that can be roughly interpreted as a coordinate free concept of singularly perturbed systems. We apply this theoretical construction for designing an algorithm that allows linear transformation of the original system into suitable SPS form. The main purposes are the simplicity (from implementation point of view) and robustness of the designed algorithm of the coordinate transformation. Moreover, properties like robustness of the procedure and consistency of the decomposed (reduced) model to the detailed one are the focus of the current results.

First, we present a more or less known algebraic procedure for a dimension reduction of stociometric matrices. Second, we present a brief outline of the coordinate free concept of singularly perturbed systems (singularly perturbed vector fields)which is a core of the suggested algorithm. After all necessary theory will be presented, the so-called Global Quasi-linearization procedure (GQL) will be described. Third, we estimate a possible dimension reduction with the help of the Global Quasi-linearization procedure. Then, some important problems of a reasonable choice of reference points for Global Quasi Linearization procedure (GQL) are discussed. A corresponding set of scalar invariants for the reference points choice is constructed. These invariant have a geometrical origin, closely connected with of the original singularly perturbed vector field and depend on the domain of interest in the phase space. Application of the algorithm are discussed in details and verified for number of model systems.

Conclusions

The main issue in this study is construction of an algorithm for a global decomposition of chemical kinetic systems with "hidden" multi-scale structure into so-called "slow" and "fast" subsystems. A robust, efficient, automatic algorithm, which is based on the Global Quasi-linearization procedure (GQL) proposed in our previous papers, has been modified for practical kinetic models in dimensional form.

Using a number of test examples it has been shown that this approach can be successfully applied numerically for the construction of linear transformations of the original models to the standard SPS form.

References

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