Efficient slow manifold identification for tabulation based adaptive chemistry

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1 Background

The dynamics of chemical kinetic systems exhibit a wide range of time scales. Computational Singular Perturbation (CSP) [1, 2] analysis facilitates the study of large and complicated reacting flow systems by decomposing the system dynamics into fast and slow dynamics. The key advantage of CSP-based reduction strategies is the ability to carry out the fast/slow decomposition automatically allowing for the replacement of a stiff system of large dimension with one which is non-stiff with a a reduced number of state variables. The numerical integration of the reduced, non-stiff model can be carried out by resorting to an explicit time-scale split integration algorithm [3]. However, a straightforward implementation of CSP is not affordable when dealing with systems of large dimension because of the high computational cost associated with the CSP analysis. One way to reduce this cost is to implement a tabulation strategy to store and reuse the manifold information generated by CSP.

Our tabulation borrows from the "Piecewise Reusable Implementation of Solution Mapping" (PRISM) [4] technique the utilization of hypercubes in the Chemical Configuration Space (CCS) and the polynomial regression of response surfaces, and adapts them to address the specific challenges of CSP, while exploiting the reduction of dimensionality offered by CSP. In contrast to conventional PRISM implementations, where the solution is mapped against the full state vector, we seek to store and reuse information of a lower, if existing, $(N-M)$-dimensional surface within the N-dimensional hypercube. Here, N is the number of unknowns in the state vector $\mathbf{y}$ and M is the number of fast time scales that, at some point in the CCS, are found "exhausted", and therefore not contributing to the (slow) dynamics of the system. Specifically, we tabulate the CSP basis vectors/covectors $\mathbf{a}$ and $\mathbf{b}$. This choice is based on the fact that the eigenvalue analysis of the Jacobian of the source term and the refinements needed for the associated computations are expensive. Moreover, the CSP vectors/covectors are at the core of the computation of important quantities such as the projection matrix $Q_s = I - \sum_{r=1,M} \mathbf{a}_r \mathbf{b}^r$ or the radical correction in the CSP integrator [3]. The implementation of the tabulation consists of building local –low-order– polynomial response surfaces of the elements of the first M columns of a and rows of b as a function of the $N-M$ active species.

The effectiveness and feasibility of the approach relies ultimately on the ability to identify the value M and the $N-M$ variables in order to characterize accurately the Slow Invariant Manifold (SIM) when the table is being constructed. and to allow for an accurate simulation of the system dynamics during integration

In this paper we show how the concept of the CSP homogeneous (radical) correction [5, 6] can be used to project any state vector picked at random in an N-dimensional hypercube onto a neighborhood of an $(N-M)$-dimensional SIM. The action of the homogeneous correction is to reduce, at each application, the amplitudes of the M fastest modes, thus monitoring the approach of the state vector to the SIM. We will adopt the definition of homogeneous (radical) correction used in [3], that is:

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$$\delta\mathbf{y} = -\sum_{m,n=1}^{M} \mathbf{a}_m \tau_n^m f^n \tag{1}$$

where $\delta\mathbf{y}$ is the displacement of the state vector in the fast subspace produced by non-vanished fast mode amplitudes $\{f^n = \mathbf{b}^n \cdot \mathbf{g}\}_{n=1}^{M}$, with $\mathbf{g}$ denoting the right hand side (RHS) of the kinetic model.

During the tabulation stage, this property is used to compute M inside the hypercube when this is sufficiently small such that any point is "close" to the manifold, and is attracted to it along the fast directions. The selection of the proper size of the hypercube is carried out adaptively during the table construction, although this issue is not discussed in this paper. By projecting the state vector onto the SIM during the integration stage, important computational savings can be achieved since the exhausted fast scales are eliminated and the number of time steps needed to accurately integrate the slow dynamics of the original system of differential equations is significantly smaller.

2 CSP "homogeneous correction"

Typically, a state vector y landing in a hypercube where a SIM of unknown dimension $(N-M)$ exists, is found sufficiently off the SIM, this causing the M fastest time scales to be active and forcing the state vector to move towards the SIM. One way to identify the SIM dimension within a hypercube is to compute trajectories starting from different points in the hypercube and to monitor how many fast amplitudes are vanished when the trajectories leave the hypercube. However, computing the trajectories soon becomes prohibitively expensive.

Alternatively, one could imagine projecting the state vector onto a SIM of presumed dimension M by resorting to the homogeneous correction, Eq.(1), which allows skipping the computation of the fast dynamics. As the SIM dimension within a hypercube, we can take the largest value of M for which the projected state vector lands inside the same hypercube.

A repeated application of the homogeneous correction, for an assumed value of M, can bring the state vector arbitrarily close to the nearest $(N-M)$-D SIM. The homogeneous correction mostly affects the variables identified as CSP radicals, whereas the non-CSP radical (major species) are relatively unaffected. The ratios $\{dy_i/y_i\}_{i=1}^{N}$ monitor the relative changes of each solution component after each correction, which can be used as a stopping criterion for the homogeneous correction iterates.

Clearly, the projected state vector on the SIM is not the same as the point that the integration trajectory would reach, starting from the same initial conditions. This only occurs if the ratio $\tau_{fast}/\tau_{slow} = 0$, otherwise the two points differ by an amount which is a function of the time, Δt, elapsed to reach the SIM from the starting point. In the next section, we show with an example that this difference can be made arbitrarily small without affecting significantly the accuracy of the integration of the slow dynamics, while the computation of the large number of very small integration time steps required to describe the fast approach to the SIM is avoided.

3 Example: a 3 species kinetics problem

To illustrate the application of the homogeneous correction, we consider the 3-species kinetics problem analyzed in [2]. The right hand side of this model problem reads:

$$\mathbf{g} = \begin{bmatrix} -\frac{5y_1}{\varepsilon} - \frac{y_1 y_2}{\varepsilon} + y_2 y_3 + \frac{5y_2^2}{\varepsilon} + \frac{y_3}{\varepsilon} - y_1 \\ 10\frac{y_1}{\varepsilon} - \frac{y_1 y_2}{\varepsilon} - y_2 y_3 - 10\frac{y_2^2}{\varepsilon} + \frac{y_3}{\varepsilon} + y_1 \\ \frac{y_1 y_2}{\varepsilon} - y_2 y_3 - \frac{y_3}{\varepsilon} + y_1 \end{bmatrix}$$

The solution trajectories are asymptotically attracted towards a 1-D SIM, a line in a 3-D phase space.

$M=1$	y_1	y_2	y_3	dy_1/y_1	dy_2/y_2	dy_3/y_3	f^1	
Initial	0.97003	0.92696	0.99514				-128.35270	
1 hc	0.94726	0.97593	0.99401	0.02346	-0.05283	0.00113	2.41797	
2 hc	0.94768	0.97504	0.99403	-0.00044	0.00091	-0.00002	0.00454	
$M=2$	y_1	y_2	y_3	dy_1/y_1	dy_2/y_2	dy_3/y_3	f^1	f^2
Initial	0.97003	0.92696	0.99514				-128.35269	-11.47343
1 hc	0.97782	0.99093	0.96854	-0.00804	-0.06901	0.02673	4.59536	-0.06144
2 hc	0.97876	0.98934	0.96844	-0.00096	0.00160	0.00010	0.00275	-0.00033

Table 1: Computed values of the state vector with relative changes, and modal amplitudes before and after applying the homogeneous correction (hc).

Consider the hypercube defined by the vertex $[y_1, y_2, y_3] = [0.875, 0.875, 0.875]$ and edge lengths $[\delta y_1, \delta y_2, \delta y_3] = [0.125, 0.125, 0.125]$, plotted in Fig. 1. Small black dots represent values of the state vector selected randomly within the limits of the hypercube. For all these "experimental design" points we computed two successive homogeneous corrections for both $M = 1$ and $M = 2$. The homogeneous correction in Eq.(1) is calculated using the eigenvectors of the Jacobian of the RHS as CSP vectors. Table 1 shows the state vector after one and two corrections for the same initial point, the relative change of each component of the state vector, and the magnitude of the fast modal amplitudes.

We can observe that, when the homogeneous correction is calculated with $M = 1$, the initial points are taken within the vicinity of a 2D surface (red points in Fig. 1). This surface is a 2-D SIM where the first modal amplitude $f^1 \approx 0$. Similarly, when $M = 2$ the corrections take the experimental design points to the vicinity of a 1-D SIM, the intersection of two surfaces at which $(f^1 \approx 0 \cap f^2 \approx 0)$ (green points in Fig. 1). The trajectory found by prescribing constant time intervals for the initial point in Tab. 1 shows the behavior of the state vector under the influence of fast scales, described in the previous section and in [2]. The blue circles in Fig. 1 represent the final values of the state vector after the corrections computed with $M = 1$ and $M = 2$.

The relative changes between initial and final points of the second correction are significantly smaller than those due to the first correction, indicating convergence towards the SIM as also confirmed by the vanishing values of the fast modal amplitudes in Tab. 1. For $M = 1$, the homogeneous correction affects the elements y_1 and y_2 to a greater extent than y_3. Therefore y_3 can be labeled as a major species and both y_1 and y_2 as CSP radicals. The pointers for y_1 and y_2 are $O(0.2)$ and $O(0.8)$ respectively, whereas the CSP pointer for y_3 is three orders of magnitude smaller. For $M = 2$ the homogeneous correction affects the 3 species to the same degree. The N diagonal elements of the fast subspace projection matrix Q_m are of the same order of magnitude, $O(0.35)$, $O(0.45)$ and $O(0.20)$ for y_1, y_2 and y_3 respectively.

Figure 2 shows the evolution vs time of the 3 species using the CSP integrator [3] and fourth order Runge-Kutta (black line). We compare these results with those obtained after 1 (red) and 2 (green) homogeneous corrections calculated with $M = 2$ (shown in Tab. 1) followed by the same CSP integration. We can observe the high accuracy of the integration after the short initial periods. The number of integration steps with CSP starting from the initial point until $\log_{10}(\text{time}) = -0.75$ is 170. After one homogeneous correction, most of the short integration steps of the rapid transit period are skipped and the number of steps drops to 65. Finally, with 2 consecutive homogeneous corrections, the modal amplitudes become negligible indicating close proximity to the 1D manifold. Under these conditions CSP is especially effective filtering out the fast scales and only 1 time step is needed to integrate the system of ODE's with comparable accuracy.

4 Conclusions

The CSP homogeneous correction provides an efficient way to identify an accurate projection on a SIM of any state vector close to but off the SIM. This property can be used to identify and characterize the SIM dimension without resorting to expensive trajectory calculations. An effective dimensionality reduction is obtained as the

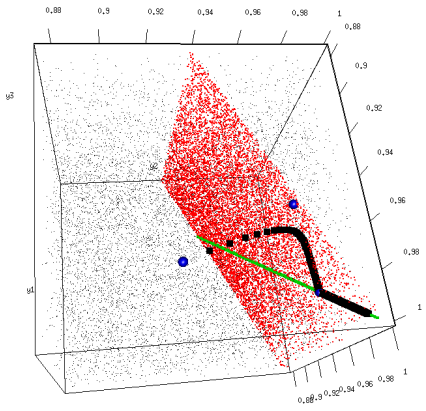

Figure 1: Black points are random design points in a hypercube defined by the vertex $[y_1, y_2, y_3] = [0.875, 0.875, 0.875]$ and edge lengths $[\delta y_1, \delta y_2, \delta y_3] = [0.125, 0.125, 0.125]$; red points calculated with $M = 1$; green points calculated with $M = 2$.

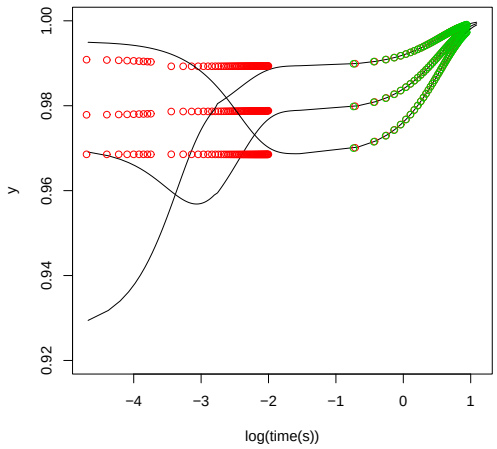

Figure 2: Time integration with CSP (black line) for an initial point $y = [0.97003, 0.92696, 0.99514]$. Red points correspond to the results of the integration after 1 homogeneous correction with $M = 2$ followed by CSP integration of the full system. Green points are the results after 2 homogeneous corrections.

CSP information can be computed as a function of just the $N - M$ major species. Significant CPU savings can be achieved by skipping the detailed calculation of the fast approach to the SIM at the cost of a minimal loss of accuracy.

Acknowledgments

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