A combined CSP-PCA framework for accelerated integration of stiff chemistry in reacting flow solvers

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1 Introduction

Numerical simulations of reacting flows are constrained by mainly two factors: large dimensionality due to the number of chemical species involved, and stiffness associated to the wide spectrum of chemical timescales. Such burden can be alleviated by the use of tabulated manifolds, where the state-space is parameterized using a reduced number of variables capable of describing the most important features of a flame. Those *a priori* tabulations lead to extensive computational savings by keeping sufficient (desirable) accuracy. However, in systems where dynamical features are of interest (such as transient phenomena, re-ignition, soot formation, etc.), direct integration of chemical ODEs is more suitable. Moreover, Direct Numerical Simulations (DNS) with detailed chemistry are often employed to investigate key features in combustion regimes operating under high Reynolds, Karlovitz and Damköhler numbers. As a consequence, these simulations either strongly limit the time-steps of explicit integration schemes, or require implicit (multi-step) integration methods which in turn increases the computational cost even further.

To mitigate the cost of stiff kinetics ODEs in flow solvers, an adaptive ODE integration explicit scheme for stiff chemistry was proposed based on the Computational Singular Perturbation (CSP) theory [1-5]. This *CSP solver* [6] exploits the existence of a local low-dimensional manifold, based on the CSP fast/slow decomposition, to adaptively remove stiffness by filtering out the fast scales from the vector of chemical source terms. The result is a set of non-stiff equations which can be integrated using explicit schemes with larger time-steps. However, the CSP solver relies on the calculation of an expensive on-the-fly basis, called the CSP projector, which is obtained from the eigensystem of the Jacobian matrix of the local chemical source term. This basis is computed at each time-step, and the associated cost can quickly become prohibitive for large mechanisms as it scales with $N^{2.5}$ to N^3, where N is the total number of species. To tackle this, the present study proposes to couple the CSP solver with Principal Component Analysis [7], and in particular to exploit the advantage offered by the Manifold Generated from PCA (MG-PCA) model [8-9]. MG-PCA allows to create a reduced-order model by identifying a subset of species which are explicitly solved, while the unresolved species are reconstructed using the

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PCA basis. By constraining the CSP solver to the subset of species identified by MG-PCA, the size of the Jacobian matrix can be reduced, accelerating the calculation of the CSP projector. The subset of ODEs can then be integrated along the MG-PCA manifold, and the remaining unresolved variables can be reconstructed at each time-step using the linear PCA basis.

2 The CSP-PCA Framework

Given any partitioning of the *N* species in two categories of *resolved* species ($\boldsymbol{u}$) of size *n* and *unresolved* species ($\boldsymbol{v}$) of size *m* (with $n + m = N$) and given a manifold $\boldsymbol{v} = F(\boldsymbol{u})$ that constrains the system to a lower-dimensional subspace, the system can be evolved in time along the reduced-order manifold (where only the resolved species are evolved in time) and subsequently, the manifold constrain is applied in order to update the unresolved species. The size of the eigensystem to be solved by the CSP solver depends on the nature of the manifold F.

If F is the CSP manifold, then the species partitioning $[\boldsymbol{u}|\boldsymbol{v}]$ is a slow-fast partitioning and therefore the source term constrained to F is freed from the fast scales. However, the identification of F requires the solution of a $(N + 1)\times(N + 1)$ eigensystem. The details on the CSP algorithm can be found in [10].

If F is any other manifold (such as the MG-PCA manifold), then the $[\boldsymbol{u}|\boldsymbol{v}]$ partitioning is not a slow-fast one, and the source term is still contaminated by fast scales. However, the dimension of such F is smaller than the full system ($n < N$), therefore reducing the computational cost associated with the eigensystem. In addition, MG-PCA has the advantage of providing a linear functional expression between the resolved and unresolved variables, $\boldsymbol{v} = F^{PCA}(\boldsymbol{u}) = \boldsymbol{u} \cdot \boldsymbol{B}$ where $\boldsymbol{B} \in \mathbb{R}^{n\times N}$ is a linear matrix. The details of the MG-PCA reconstruction are given in [11].

Constraining the Jacobian matrix to a low-dimensional manifold requires the evaluation of a *Constrained Jacobian* matrix $J_C \in \mathbb{R}^{n\times n}$ as follows:

$$J_C = \frac{\partial g_i(\boldsymbol{u},\boldsymbol{v})}{\partial u_j} + \frac{\partial g_i(\boldsymbol{u},\boldsymbol{v})}{\partial v^\alpha}\frac{\partial v^\alpha}{\partial u_j} \qquad i,j = 1,n \quad \alpha = 1,m$$

where g_i is the chemical source term of species i. The evaluation of the derivative $\partial v^\alpha/\partial u_j$ is directly obtained from the linear expression provided by MG-PCA, i.e. $\boldsymbol{v} = \boldsymbol{u} \cdot \boldsymbol{B}$.

3 Application – Homogeneous Reactor

The proposed reduced CSP-PCA model is compared to the classical (detailed) CSP in a $0D$ constant-pressure reactor using the PyCSP Python package [12]. The initial condition is a stoichiometric mixture of NH_3/air at 1400 K and 1 atm. The detailed kinetic mechanism of Zhang et al. [13] was used, consisting of 36 species and 258 reactions.

The MG-PCA training data was generated using the same setup by varying the initial temperature from 1400 K to 1500 K. The final data set contained 50,000 observations for each of the state-space variables. All of the data points were used collectively for the PCA analysis. Using the B2 backward selection method [14] with pareto scaling [15], 22 species were identified that would allow for a quasi-exact reconstruction of the other species. In MG-PCA, the minimum number of retained species is constrained by the reconstruction accuracy of the discarded species.

The detailed CSP is therefore based on a Jacobian of size (36+1), while the reduced model has a constrained Jacobian of size (22+1).

3.1 Timescales analysis

Figure 1 shows the eigenvalues (inverse of timescales) of the full and reduced model for the $0D$ reactor. The $(M+1)$-th eigenvalue evolution is also shown in orange, where M is the number of exhausted modes representing the fast timescales of the system (the lower M, the faster the chemical activity). The $(M+1)$-th eigenvalue therefore represents the fastest timescale of the slow dynamics, which determines the integration time-step. Indeed, as explained in [10], the larger M, the smaller the number of truly active (slow) degrees of freedom, the larger the time-step can be. The fast/exhausted eigenvalues are the ones above the orange line on Fig. 1. The magnitude of the $(M+1)$-th eigenvalue changes in time according the value of M. It can be observed on Fig. 1 that the reduced model depicts a lower $(M+1)$-th eigenvalue (higher M) compared to the full model during some regions of the time evolution, namely in the initial phase and after ignition (steady-state). A higher M implies a lower number of active modes, therefore allowing for larger integration time-steps.

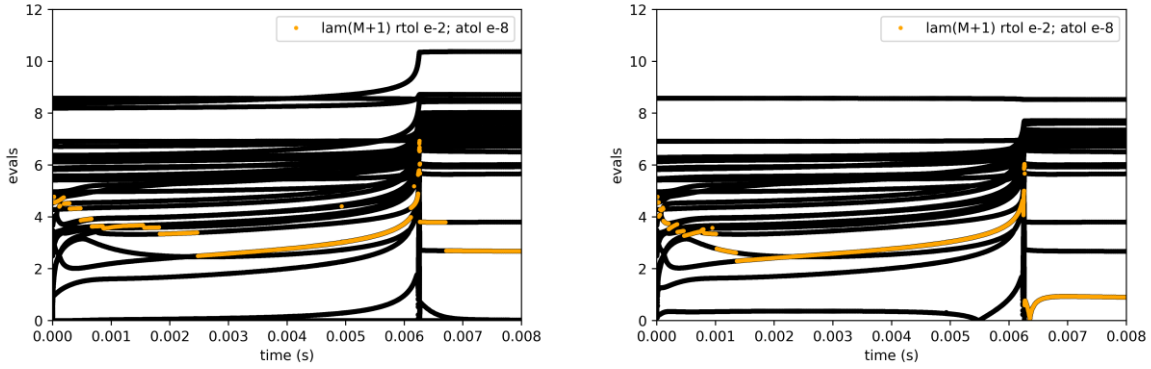

Figure 1: Eigenvalues (black) and $(M+1)$-th eigenvalue (orange) against time for the detailed CSP (left) and reduced CSP-PCA (right) systems.

3.2 Results

The performance of the reduced CSP-PCA model are compared against the full model inside the CSP solver in PyCSP. Figure 2 shows the evolution of temperature and OH mole fraction in function of time for the $0D$ reactor initiated with $T = 1400\ K$. It can be seen that the reduced model is able to capture the transient evolution of the system, showing a very good agreement with the full CSP model.

Figure 3 (left) shows the variation of the relative number of exhausted modes M_{rel} (defined as $M/total\ number\ of\ variables$) during the time evolution for the detailed and reduced models, while Fig. 3 (right) shows the evolution of the integration time-step. M_{rel} is higher for the reduced CSP-PCA model for most of the simulation, confirming the observation made above (Fig. 1). The reduced model also allows for larger integration time-steps in some parts of the simulation, leading to a reduction in the overall CPU time. Table 1 reports the total CPU time for both cases, showing that the reduced model is able to achieve a reduction of $\sim 40\%$ in solver time. This reduction is mainly due to the reduction in size of the Jacobian matrix (and therefore also of the eigensystem), and also to some extent to the larger integration time-steps in some regions of the simulation.

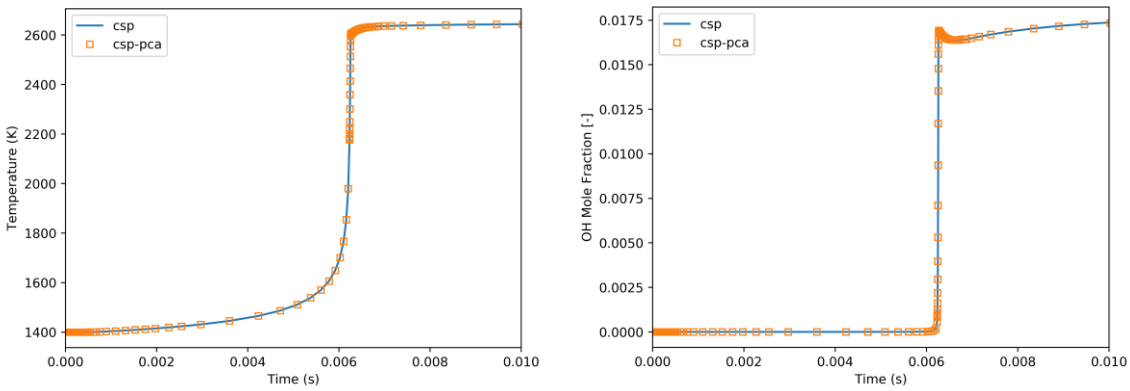

Figure 2: Temperature (left) and OH model fraction (right) in function of time for the full CSP case (line) and the reduced CSP-PCA model (symbols).

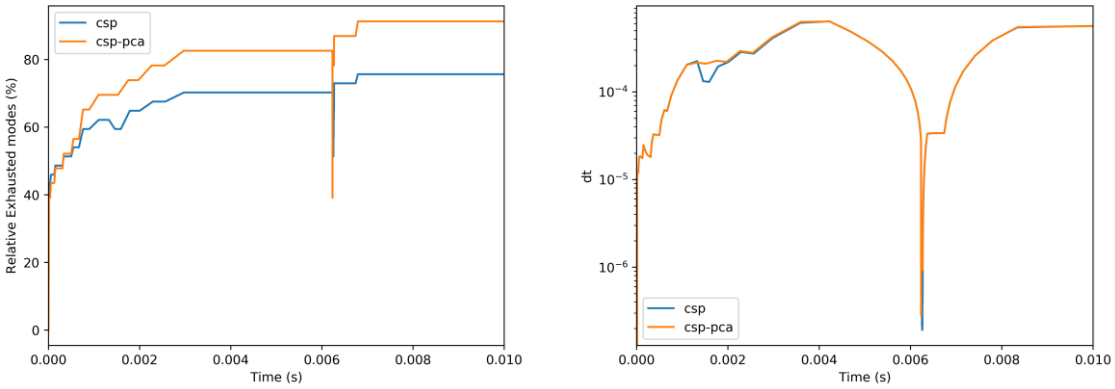

Figure 3: Relative number of exhausted modes M (left) and integration time-step (right) in function of time for the full CSP case (blue) and the reduced CSP-PCA model (orange).

Table 1: Total CPU time for the full (CSP) and reduced (CSP-PCA) simulations.

Model	Total solver time [s]
CSP	0.698
CSP-PCA	0.412

In summary, constraining the CSP solver to a reduced-order manifold identified using PCA allows the solver to work in a reduced dimension space ($n < N$). The cost of the eigensystem calculation is therefore alleviated, but since the PCA manifold is not equal to the CSP manifold, the reduced system still relies on an internal fast/slow decomposition. Nevertheless, the reduced CSP-PCA model allows for a significant CPU time reduction while maintaining good accuracy in the prediction of state-space variables.

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