Relaxation Redistribution Method for model reduction

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***Abstract*— The Relaxation Redistribution Method (RRM) is based on the notion of slow invariant manifold (SIM) and is applied for constructing a simplified model of detailed multiscale combustion phenomena. The RRM procedure can be regarded as an efficient and stable scheme for solving the film equation of dynamics, where a discrete set of points is gradually relaxed towards the slow invariant manifold (SIM). Here, the global realization of the RRM algorithm is briefly reviewed and used for auto-ignition and adiabatic premixed laminar flame of a homogeneous hydrogen-air ideal gas mixture.**

I. Introduction

The detailed reaction mechanisms of practical fuels contain hundreds of species participating in hundreds to thousands of elementary chemical reactions. In addition to the large number of variables that need to be accounted for, disparate time scales introduce stiffness and increase the computational cost of numerical computations. On the other hand, time scales associated with transport phenomena cover a narrower range of typically slower time scales. When the coupling of flow phenomena and chemical kinetics is of interest, changes due to the fastest time scales can be assumed to be equilibrated. Model reduction can then be employed to reduce the computational cost by extracting only the important slow system dynamics [1], [2], [3].

The *Relaxation Redistribution Method* (RRM) was recently proposed as an efficient technique to construct low dimensional manifolds of any dimensions [4]. RRM consists of an algorithm for refining an initial guess (initial grid) till convergence within a neighborhood of the SIM is achieved, by mimicking the film equation of dynamics. Here, the initial manifold is immersed into a phase space and the motion of trajectories along the manifold is subtracted from the whole dynamics by a simple redistribution of the grid points in the reduced space. Moreover, in its local realization, stability of the RRM refinements provide a natural criterion for finding the minimal dimension of a reduced model [4].

Here, the global realization of RRM is shortly reviewed and applied for homogeneous auto-ignition and a laminar premixed hydrogen flame.

II. Film equation of dynamics and RRM

The detailed (microscopic) dynamics of an autonomous system in terms of the state $\mathbf{N}(t)$ in a phase space S (say n_s-dimensional) is given by,

$$\frac{d\mathbf{N}}{dt} = f(\mathbf{N}). \tag{1}$$

A subspace $U \subset S$ is a positively invariant manifold for the system (1) if every trajectory starting on U at time t_0 remains on U for any $t > t_0$. Therefore, $\mathbf{N}(t_0) \subset U$ implies $\mathbf{N}(t) \subset U$ for $t > t_0$.

The components of the state vector typically evolve at different time scales. Because of such time scale disparity, the trajectories of (1) starting from arbitrary initial conditions are typically quickly attracted to a lower dimensional manifold, where motions continue at a slower rate towards the steady state (or equilibrium $\mathbf{N}^{eq}$ with $f(\mathbf{N}^{eq}) = 0$). This positively invariant manifold is the *slow invariant manifold*, (SIM), and its construction can be based on the definition of fast and slow sub-spaces within S [3].

Accordingly, neglecting the initial fast evolution of the detailed system, the long-time dynamics can be described by a smaller number of macroscopic variables, which are to be used to *uniquely* parametrize the SIM. The macroscopic variables $\boldsymbol{\xi}$ belong to the n_d-dimensional space Ξ, with $n_d < n_s$, and offer a possible representation for a coarse description of (1). In other words, for an arbitrary state $\mathbf{N}^{SIM}$ located on the low-dimensional manifold, we can write $W = \mathbf{N}^{SIM}(\boldsymbol{\xi})$, where W is a $(1-1)$ map from the parameter space Ξ into the phase-space S.

The evolution rate of the state $\mathbf{N}$, $f(\mathbf{N})$, can be decomposed into a component along the tangent space of W, T_W, and its complement in a transversal direction,

$$f(\mathbf{N}(\boldsymbol{\xi})) = f(\mathbf{N}(\boldsymbol{\xi}))_{\|_{T_W}} + f(\mathbf{N}(\boldsymbol{\xi}))_{\perp_{T_W}}, \tag{2}$$

The components are defined as

$$f(\mathbf{N}(\boldsymbol{\xi}))_{\|_{T_W}} = \mathbf{P} f(\mathbf{N}(\boldsymbol{\xi})) \tag{3}$$

$$f(\mathbf{N}(\boldsymbol{\xi}))_{\perp_{T_W}} = \Delta = (\mathbf{I} - \mathbf{P}) f(\mathbf{N}(\boldsymbol{\xi})). \tag{4}$$

Δ is the *defect of invariance* where $\mathbf{I}$ and $\mathbf{P}$ are $n_s \times n_s$ identity matrix and projector operator, respectively.

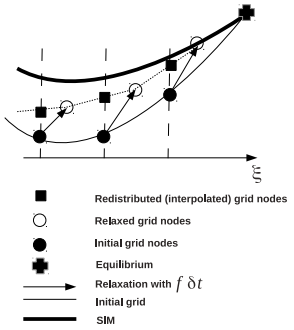

Fig. 1. Relaxation and Redistribution algorithm; The effect of slow motions is neutralized via redistribution.

By definition, W is a positively invariant manifold if the state does not leave it during the subsequent system evolution. Hence, relaxation will happen only along the tangent space and the normal component should be zero,

$$\Delta = 0 \qquad \boldsymbol{\xi} \in \Xi. \tag{5}$$

Equation (5) is the differential equation which is known as *invariance condition* [3]. In the *Method of Invariant Manifold* (MIM), the slow invariant manifold is the stable solution of the film extension of dynamics, $\frac{d\mathbf{N}(\boldsymbol{\xi})}{dt} = \Delta$. This is the evolutionary equation guiding an initial mapping $\mathbf{N}(\boldsymbol{\xi})$ towards $\mathbf{N}^{SIM}(\boldsymbol{\xi})$. A detailed explanation of MIM algorithm and the choice of the projector $\mathbf{P}$ can be found in [5], [6].

The states located on an initial grid relax according to (1) with $f(\mathbf{N}^{ini}(\boldsymbol{\xi}))$. After some time, all grid points move towards the SIM and the volume of the initial manifold shrinks due to the concurrent action of slow motions. In the RRM though, the latter effect is neutralized by redistributing the points of the relaxed grid after each time step [4]. As sketched in Fig. 1, relaxed grid (open circles) are located at different positions on the slow space Ξ with respect to their initial positions (black circles). Clearly, even after a short relaxation the density of the grid points tends to increase near the equilibrium, with a drastic change of the grid spacing in Ξ. To prevent this, a redistribution step is applied to bring the grid points back to their previous ξ values. Such a step requires interpolation between the inner relaxed states and extrapolation for boundary grid points. The converged solution is the manifold containing all the states for which further relaxations move the states only along the manifold. In order to keep the computational effort low, here we focus on manifolds with a dimension up to three. We should however remind that low dimensional SIM are usually appropriate within some neighborhood of the phase space around the equilibrium point, leaving open the problem of how to extend it further to cover the states all the way to the fresh mixture condition [7].

On the other hand, in the original RRM method, extrapolations during the redistribution step at the SIM boundaries may sometimes result in physically meaningless values for compositions (e.g. negative concentrations). In this work, to prevent such a problem, we suggest a possible approximate solution as follows. Global 2D or 3D initial manifolds are constructed (see RCCE construction below) and their boundaries subsequently fixed during the refinement process. In other words, the RRM is applied just on the interior grid points till convergence. Based on our experience, the resulting manifold practically coincides with the SIM for the part of the phase space for which low dimensional SIM exists, whereas it provides with a convenient extension for regions far from equilibrium.

III. Results

The global RRM method is applied to homogeneous H_2/air mixtures. The detailed kinetics scheme includes $n_s = 9$ species and 21 reactions [8]. The popular *Rate-Controlled Constrained-Equilibrium* (RCCE) linear constraints (see e.g. [9]) are used for manifold parameterization, such as the total number of moles (ξ_1), moles of active valences (ξ_2) and moles of free oxygen (ξ_3).

The initial mole numbers of the species are given based on stoichiometric values, $N_{\mathrm{H_2}} = 1.0$, $N_{\mathrm{O_2}} = 0.5$ and $N_{\mathrm{N_2}} = 1.881$. The rest of the species are assigned chemically insignificant positive initial values to ensure a strictly positive composition [10]. The initial guess for the manifold (initial grid) is constructed on Ξ as much extent as possible to contain both projected locations of initial and equilibrium points. The initialization is done based on constrained minimization of thermodynamic potentials utilizing the CEQ FORTRAN package library [11].

The grid points which are located on the boundaries are fixed and global RRM procedure applied for interior grid. The SHEPPACK FORTRAN package is used for interpolation [12]. The RCCE and RRM manifold are shown in Fig. 2 while the sample trajectory is plotted for comparison. The temporal evolution of the temperature and species mass fractions are presented in Fig. 3. Good agreement is found with the detailed description for the temperature and major reactants as well as the radicals in large concentration. Far away from equilibrium, the RCCE manifold results in strongly underpredicted HO_2 and H_2O_2 concentrations.

At the Workshop, results will be presented for the test case of a laminar premixed hydrogen flame.

IV. Conclusion

An algorithm for constructing the globally generated manifold is proposed based on the relaxation and redistribution method. The accuracy of the method has been assessed through the auto-ignition and laminar premixed flame of homogeneous H_2/air from the initial mixture far from equilibrium. The proposed method shows the improvements for ignition delay and capturing the radicals with respect to the popular low dimensional RCCE method.

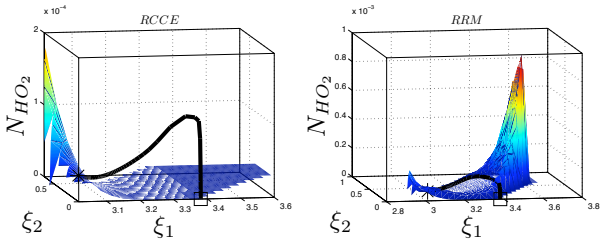

Fig. 2. RCCE and RRM manifold with the detailed system trajectory. ξ_1 is the number of total moles and ξ_2 is the moles of free valence.

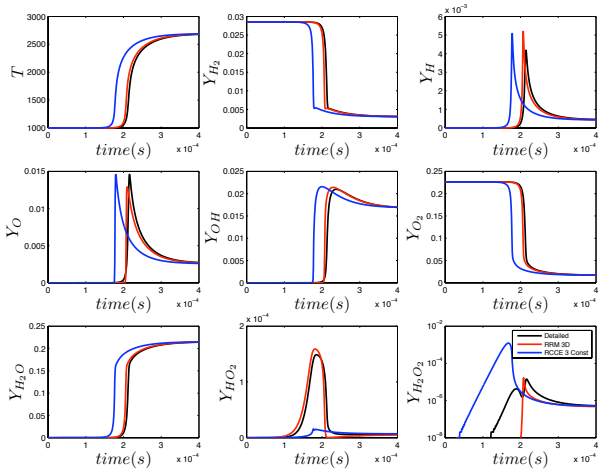

Fig. 3. Temporal evolution of species and temperature found by 3-dimensional RCCE and RRM manifolds for stoichiometric H_2/air with T_0 = 1000 K

V. ACKNOWLEDGMENTS

This work is supported by Swiss National Foundation under Project number 137771. I.V. Karlin thanks support of ERC Advanced Grant ELBM. E. Chiavazzo acknowledges support of the Fulbright commission.

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