Simplication of reactive systems by the Relaxation Redistribution Method (RRM)

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Eliodoro Chiavazzo*, Ilya Karlin†,‡
*Politecnico di Torino/Department of Energetics, Torino, Italy
†Swiss Federal institute of technology/Aerothermochemistry and Combustion Systems Lab, Zurich, Switzerland
‡University of Southampton/School of Engineering Sciences, Southampton, UK

***Abstract*—We review the novel Relaxation Redistribution Method (RRM) for the construction of accurate discrete approximations of slow invariant manifolds. Both formulations (global and local) are discussed. A fully adaptive local formulation, with a simple implementation in any dimension, is worked out and illustrated with an example of autoignition of the hydrogen-air mixture.**

I. Introduction

Detailed reaction mechanisms of combustion of hydrocarbon fuels are prototypical examples of complex dissipative systems. In this respect, modern research typically has to cope with an increasing difficulty mainly in two aspects: First, the number of degrees of freedom is tremendously large; second, complex system dynamics is characterized by a wide range of time-scales. As a result, the usage of detailed reaction mechanisms in the reactive flow simulation soon becomes intractable even for supercomputers, as for example in the turbulent combustion of even simplest fuels such as hydrogen [1]. Thus, there is a demand for methodologies capable of both drastically reducing the description of complex systems with a prohibitively large number of variables, and concurrently allowing new physical insights to be gained.

II. Method of invariant manifold

Let the detailed description be given by an autonomous system in terms of the state ψ on a phase space U with a unique steady state,

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

Important example of (1) to be addressed below is the reaction kinetics where $\psi = \left(\psi^1, \ldots, \psi^n\right)$ is a n-dimensional vector of concentrations of various species while the vector field f is constructed according to the detailed reaction mechanism and (usually) the mass action law. A consistent approach to model reduction is provided by the Method of Invariant Manifold (MIM) in the formulation of Gorban and Karlin [4] which we first briefly review. In MIM, the problem of model reduction is identified it with the construction of a slow invariant manifold (SIM) $\Omega_{\rm SIM}$. A sub-manifold Ω (not necessarily a SIM) is embedded in the phase space U and is represented by a function $F(\xi)$ which maps a macroscopic variables space Ξ into U. Introducing a projector P onto the tangent space T of a manifold Ω (not necessarily invariant), the reduced dynamics on it is defined by the projection $Pf(\Omega) \in T$. A manifold Ω is termed invariant (but not necessarily *slow*) if the vector field f is tangent to the manifold at every point: $f(F(\xi)) - Pf(F(\xi)) = 0$. While the notion of a manifold's invariance is relatively straightforward, a definition of slowness is more delicate as it necessarily compares a (faster) approach towards the SIM with a (slower) motion along SIM. In MIM, slowness is understood as stability, and SIM is a stable fixed point $F_{\rm SIM}(\xi)$ of the *film equation* defined on the space of maps F [4],

$$\frac{dF(\xi)}{dt} = f(F(\xi)) - Pf(F(\xi)). \tag{2}$$

Motion separation in a vicinity of SIM is dictated by projector P: Slow motions along SIM are locked in the image, $\mathrm{im}P = T$, whereas the null-space spans the fibers of fast motions transversal to SIM. Rigorous proofs of existence and uniqueness of SIM, by the film equation (2), were recently given for linear systems [7]. A natural approach to the construction of SIM's is a direct numerical solution of the film equation (2) starting with an initial manifold (grid). For that, both the initial condition as well as implicit or semi-implicit schemes were developed. However, the latter methods usually attempt the construction of invariant manifolds, in the whole phase-space, by assigning *a priori* their dimensionality q somewhat arbitrarily. Such an approach, where the parameter q does not arise from the system but rather comes as *external input* into the problem, poses severe limitations on the accuracy of the reduced description and, most detrimentally, hinders the gaining of a better physical knowledge about it. Moreover, construction of high-dimensional invariant manifolds ($q \geq 3$) by the direct solution of the equation (2) has revealed quite problematic and never successfully accomplished up to now.

III. RRM: Global construction

A novel relaxation method, based on the rationale behind Eq. (2), for grid refinements has been recently introduced [2], [3]. For illustration purposes, we refer to a one-dimensional initial grid $\mathcal{G}_0$, schematically drawn in Fig. 1, as a discrete analog of one-dimensional manifold. Let $\mathcal{G}_0$ be chosen regular in terms of a parameter ξ.

Let all grid nodes relax towards the slow invariant manifold (SIM) under the detailed dynamics f during

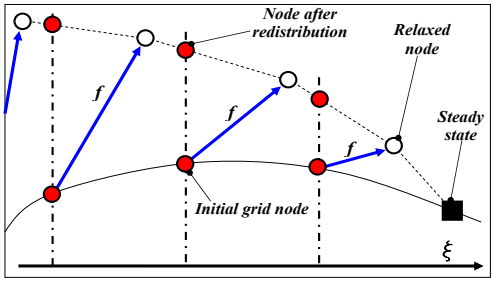

Fig. 1. One refinement step by the Relaxation Redistribution Method (global approach).

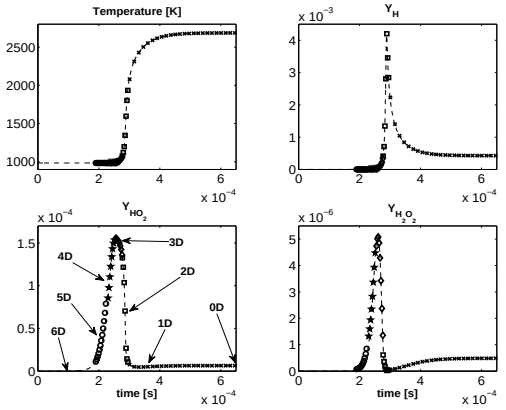

Fig. 2. Comparison between detailed (continuous line) and reduced models (symbols) for auto-ignition of hydrogen and air. The RRM method (local formulation) adaptively choses the dimension of the reduced description: From 0D (steady state) up to 6D (full dimensionality).

one time step: The fast component of f brings a grid node closer to the SIM while, at the same time, the slow component causes a contraction towards the steady state. As a result, the grid becomes dense in a neighborhood of the steady state and coarse far from it, when keeping relaxing. Nevertheless, the slow motion can be neutralized by a node redistribution after the grid relaxation. In other words, as illustrated in Fig. 1, the relaxed states are redistributed on a regular grid in terms of the parameter ξ.

All intermediate grids are, by construction, regular in terms of ξ and, in the case of an invariant grid, the overall effect due to relaxation and redistribution is null. In other words, the movement (due to relaxation) of a node along the slow subspace is perfectly compensated by the subsequent redistribution step. Therefore, a measure of the invariance defect is now given by the overall motion of a node (relaxation + redistribution) compared to relaxation alone. By analogy with the MIM method, an invariant grid represents the *stable* fixed solution of the described procedure, whose name is *relaxation redistribution method* (RRM). It is worthy stressing that the above methodology does not make explicit use of a projector P on the tangent space of $\mathcal{G}_0$. On the contrary, the role of P is now played by the redistribution sub-step after the relaxation: As a consequence, significantly stable iterations (compared to direct solution of (2)) are observed.

IV. RRM: Local construction

Both construction and usage of *global reduced descriptions* soon become impracticable, as the degrees of freedom q increase, since computing and storage of high dimensional manifolds may be pretty problematic, even with $q \geq 3$. Above all that, data retrieval by interpolation on such large arrays is computationally intensive, and sometimes full construction of manifolds can be useless: For example, regions with high concentration of radicals are highly unlikely to be visited. In general, what is required in model reduction is the mapping of a macro-state ξ into a micro-state $F(\xi)$ of the phase-space U (*closure problem* of the reduced model). In this perspective *local approaches* are more appealing, because they provide a closure without generating the whole of the manifold (or significant portions of it). Hence, besides the above global construction, a *fully adaptive* local formulation of the RRM has been developed in any dimension: In fact, it has been proven that the latter procedure is able to dynamically chose, up to any dimension, among a hierarchy of reduced descriptions characterized by an increasing number of degrees of freedom q [3]. In Figure 2, we consider the auto-ignition of a stoichiometric mixtures of hydrogen and air, reacting according to the detailed mechanism [5], in a closed reactor with fixed pressure and enthalpy. We report the comparison between the detailed and reduced solution: Stability of the RRM iterations can be used for evaluating the manifold dimension. As shown, low dimensional reduced models ($q < 3$) are suitable only close to the steady state.

The latter methodology can be used within a reactive flow solver for the *real time* computing of states on a slow invariant manifold: In that case a valuable speed-up can be achieved by combining it with smart storage-retrieval methodologies such as *in situ* adaptive tabulation (ISAT) [6].

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