Adaptive Model Reduction and the G-Scheme

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***Abstract*— The numerical solution of mathematical models for reaction systems in general, and reacting flows in particular, is a challenging task because of the simultaneous contribution of a wide range of time scales to the system dynamics. However, the dynamics can develop very slow and very fast time scales separated by a range of active time scales. We propose a numerical technique consisting of an algorithmic framework, named the *G-Scheme*, to achieve multi-scale adaptive model reduction along-with the integration of the differential equations (DEs). We assume that the dynamics is decomposed into active, slow, fast, and when applicable, invariant subspaces. Adjusting the active DEs dynamically during the time integration is the most significant feature of the *G-Scheme*, since the numerical integration is accomplished by solving a number of DEs typically much smaller than the dimension of the original problem. To demonstrate the effectiveness of the *G-Scheme*, we present results from an illustrative problem.**

I. Introduction

Solutions of reaction systems in general are computationally very expensive because of the presence of a very large range of scales. However, to within an arbitrary but fixed accuracy, there are in general vary fast and very slow time scales whose contributions to the active dynamics is small. Recently, we proposed a new methodology [1] that exploits this dynamic behavior to design a numerical framework able to achieve adaptive reduction of the dynamical system based on accuracy requirements. As a result, the original problem not only becomes substantially smaller, but more importantly non-stiff. The frozen (slow) and near-equilibrium (fast) modes play crucial roles in defining the active (dynamic) subspace, and thus it is mandatory to account for their contributions. In this work, we provide an overview of the *G-Scheme* and present results of an illustrative low dimensional system to demonstrate the effectiveness of the method.

II. Basic Concepts

The present work deals with model reduction concepts that are used to develop a time accurate computational tool that is able to exploit, adaptively, opportunities for reduction from both fast/active and slow/active spectral gaps. [1] The class of multi-scale problems which can be efficiently addressed with the new framework is that of stiff problems characterized by fast time scales of dissipative nature. Operationally, the new framework is designed to deal with the same class of problems as those handled efficiently by BDF methods.

The proposed numerical technique consists of an algorithmic framework, that for convenience will be referred to as the *G-Scheme*, to achieve model reduction along-with the numerical integration of a set of **d**ifferential **e**quations (DEs). The method is directly applicable to initial-value **o**rdinary **d**ifferential **e**quations (ODEs), and by using the method of lines to **p**artial **d**ifferential **e**quations (PDEs) as well. We describe the *G-Scheme* as a "framework", since the scheme consists of a modular procedure, where several of its components can be replaced or improved, while the overall framework remains unchanged, and can be used in different ways to achieve different goals.

The rationale used in constructing the *G-Scheme* is as follows [1]. The construction of reduced models for a dynamical system whose asymptotic behavior might involve fixed equilibrium points, or nontrivial limit sets, such as limit cycles or chaotic attractors, is strictly related to the occurrence of a gap in the spectrum of its characteristic time scales (time-scale separation). A temporal gap separates fast modes relaxing towards a SIM from the slow modes that drive the system, whereas for systems possessing nontrivial invariant limit sets, the temporal dichotomy is between stable and unstable modes. In both cases, the most relevant asymptotic behavior of the system is confined to an invariant set which is attracting: the SIM or the limit attractor.

The characterization of the local structure of these invariant subspaces can be of great importance in the development of methods aimed at achieving a low-dimensional description of dynamical systems. The basic idea is that the invariant subspaces, ordered in a decreasing way with respect to their characteristic time scales, provide the most convenient and natural basis for describing the unstable/slow and stable/fast components of the dynamics. Consequently, model reduction can be achieved by filtering out the dynamically irrelevant degrees of freedom associated with the most stable (fast) components characterized by the most negative characteristic time scales.

Ideally, one would like to decompose the tangent space $\mathcal{T}_x$ at any point $\mathbf{x} \in C \subset \mathbb{R}^N$ in N invariant subspaces, so that the dynamics within each invariant subspace is fully decoupled from all other invariant subspaces, and is associated with a single characteristic time scale. This goal is not easy to achieve. However, decomposing the tangent space in subspaces, not necessarily invariant, characterized by time scales of comparable magnitude is at the core of the *G-Scheme* [1]. We assume that the tangent space $\mathcal{T}_x$ can be decomposed as the sum of four subspaces,

$$\mathcal{T}_x = \mathbb{E} \oplus \mathbb{H} \oplus \mathbb{A} \oplus \mathbb{T},$$

where the active subspace $\mathbb{A}$ contains all the current

intermediate dynamic time scales, all scales faster and slower than the active ones are confined in the fast and slow subspaces $\mathbb{T}$ and $\mathbb{H}$, respectively, and, $\mathbb{E}$ is the linear subspace spanned by directions associated with invariants, if any exist.

At each state point $\mathbf{x}$ corresponding to time t, the *G-Scheme* introduces a curvilinear frame of reference, defined by a set of orthonormal basis vectors with corresponding coordinates, attached to the decomposition of the tangent space in the four subspaces. At any time instant of the system evolution, the curvilinear coordinates are suitable (linear) combinations of the perturbations $\Delta\mathbf{x}$ of the original state vector $\mathbf{x}$ about $\mathbf{x}$ itself, which are assumed to be valid only within a time scale suitably defined. Thus, they can be thought of as "lumped" variables dynamically adjusting to the system's evolution.

The evolution of the curvilinear coordinates associated with the subspace $\mathbb{A}$ is described by $N_A = \dim(\mathbb{A}) \leq N$ ODEs, whereas the variation of the curvilinear coordinates associated with the subspaces $\mathbb{T}$ and $\mathbb{H}$ are accounted for by applying $N_T = \dim(\mathbb{T}) \geq 0$ and $N_H = \dim(\mathbb{H}) \geq 0$ algebraic corrections derived from asymptotics of the original ODEs. Note that if we have $N_E = \dim(\mathbb{E}) \geq 0$ invariants, they can be formally eliminated so that the dynamics is restricted to move in the subspace $\mathbb{H} \oplus \mathbb{A} \oplus \mathbb{T}$ that satisfies the invariants exactly. Adjusting the active ODEs dynamically during time integration is the most significant feature of the *G-Scheme*, because the numerical integration of the state vector $\mathbf{x} \in \mathbb{R}^N$ is obtained by solving a number of ODEs typically much smaller than N. The active ODEs evolve in $\mathbb{A}$, which is freed from fast scales, and thus they are non-stiff. They can be solved by resorting to any explicit time integration scheme (*e.g.*, ERK). When compared to a standard BDF implicit scheme for stiff problems, the *G-Scheme* offers the advantage of requiring the solution of $N_A \ll N$ explicit instead of N implicit ODEs, at the expense of identifying the time scales and computing the set of orthonormal basis vectors that define the curvilinear frame of reference.

A. Basis Vectors and Time Scales

Clearly, the success of the *G-Scheme* relies on the ability to identify a decomposition of $\mathcal{T}_x$ which ensures minimal (ideally no) coupling among slow, fast, and active subspaces. The problem of finding a frame of reference yielding the maximal degree of fast/slow decoupling can be approached by resorting to the CSP refinements procedure [2]. In this work, we identify the set of basis vectors $\mathbf{a}_i$, defining the mapping of the change of frame of reference, with the right eigenvectors of the Jacobian matrix J of the vector field related to the problem of interest, with the dual vectors $\mathbf{a}^j$ coinciding with the left eigenvectors of J. This yields a leading order approximation of the CSP vectors [3]. As estimate of the characteristic time scales, we consider the reciprocal of the eigenvalues, λ_i, of J. The ordering of the basis vectors is critical for proper decomposition. Here, we order the modes according to the magnitude of the complex eigenvalues, that is

$$0 = |\lambda_1| = \cdots = |\lambda_E| < |\lambda_{E+1}| < \cdots < |\lambda_{H-1}| \ll |\lambda_H| < \cdots < |\lambda_T| \ll |\lambda_{T+1}| < \cdots < |\lambda_N|,$$

where

$$\begin{aligned} 0 = |\lambda_1| = \cdots = |\lambda_E| &\quad \text{identify the time scales in } \mathbb{E}, \\ |\lambda_{E+1}| < \cdots < |\lambda_{H-1}| &\quad \text{identify the time scales in } \mathbb{H}, \\ |\lambda_H| < \cdots < |\lambda_T| &\quad \text{identify the time scales in } \mathbb{A}, \\ |\lambda_{T+1}| < \cdots < |\lambda_N| &\quad \text{identify the time scales in } \mathbb{T}, \end{aligned}$$

with $N_E = E$, $N_H = H - E - 1$, $N_A = T - H + 1$, and $N_T = N - T$. Note that, because of this ordering, (possibly complex) eigenvalues with both negative and positive real parts can be found in $\mathbb{H}$ and $\mathbb{A}$, whereas we expect the eigenvalues in $\mathbb{T}$ to have dominant negative real parts. This is the distinguishing feature of the class of problems for which the *G-Scheme* is expected to perform efficiently. The ratios $\epsilon_T \equiv |\lambda_T/\lambda_{T+1}| < 1$ and $\epsilon_H \equiv |\lambda_{H-1}/\lambda_H| < 1$ are measures of the spectral gaps between active and fast subspaces, and slow and active subspaces, respectively. Since the *G-Scheme* approximates the contribution of the very slow and very fast time scales with asymptotic corrections, it is expected that its accuracy and efficiency will be higher for larger spectral gaps, that is for smaller values of ϵ_T and/or ϵ_H. The controlling (driving) time scale of the dynamics is given by the fastest of the (active) time scales present in $\mathbb{A}$, and will be of the order of $\tau_T = 1/|\lambda_T|$.

III. The *G-Scheme*

Consider the Cauchy problem defined by a set of autonomous ODEs:

$$\frac{d\mathbf{x}(t)}{dt} = \mathbf{f}(\mathbf{x}(t)),$$

with $\mathbf{x} \in \mathbb{R}^N$, and $\mathbf{f} : E \subset \mathbb{R}^N \to \mathbb{R}^N$. We wish to find the numerical solution for $t \in (t_0, t_f]$ with given initial condition $\mathbf{x}(t_0) = \mathbf{x}_0$.

The state vector $\mathbf{x}(t)$ at time $t = t_n + \tau$, with $\tau \in \Omega \equiv (0, \Delta t] \subset \mathbb{R}$, where $\Delta t = (t_{n+1} - t_n)$, can always be expressed as the sum of the state vector $\mathbf{x}(t_n)$, for $n = 0, 1, 2, \ldots$, and a perturbation vector $\Delta\mathbf{x}(\tau)$. We note that t_n is some fixed arbitrary time. The component-wise representation of the perturbation vector $\Delta\mathbf{x}(\tau)$ can be expressed in terms of curvilinear coordinates $\Delta\mathbf{x} = \Delta\xi^i\mathbf{a}_i = \Delta\xi_j\mathbf{a}^j$ related to the sets of orthonormal covariant and contravariant basis vectors $\mathbf{a}_i$ and $\mathbf{a}^j$, respectively, here taken to correspond to the eigenbases of

$$J(\mathbf{x}(t)) \equiv \left[\frac{\partial\mathbf{f}}{\partial\mathbf{x}}\right]_{\mathbf{x}(t)}.$$

We take a curvilinear frame of reference that varies with time. If the system is autonomous, then the frame of reference depends only on the state of the system.

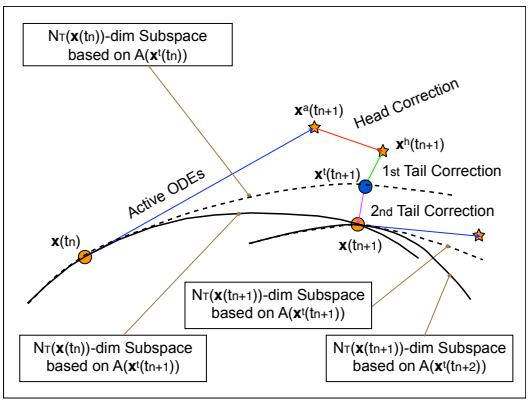

Fig. 1. The *G-Scheme* step-by-step starting from a given state $\mathbf{x}(t_n)$ on a subspace of dimension evaluated at t_n: orange stars denote intermediate new states before the application of head or tail corrections, the blue circle denotes the new state after head and tail corrections onto the subspace evaluated at t_n and where the basis vectors are subsequently updated to t_{n+1}, orange circle denotes the new state $\mathbf{x}(t_{n+1})$ and the location where the subspace dimension possibly changes. Note that in reality the orange circles are not exactly on the SIM; we're actually calculating the ASIM. We do not show both the SIM and ASIM so as not to make the figure unduly complex.

Subsequently, we can write

$$\begin{aligned}\mathbf{x}\,(t) &= \mathbf{x}_n + \Delta\mathbf{x},\\ &= \mathbf{x}_n + A_e\,\Delta\boldsymbol{\xi}^e + A_h\,\Delta\boldsymbol{\xi}^h + A_a\,\Delta\boldsymbol{\xi}^a + A_t\,\Delta\boldsymbol{\xi}^t,\\ &= \mathbf{x}_n + \Delta\mathbf{x}^e + \Delta\mathbf{x}^h + \Delta\mathbf{x}^a + \Delta\mathbf{x}^t,\end{aligned}$$

where

$$A(\tau) \equiv [\mathbf{a}_1(\tau)\ \cdots\ \mathbf{a}_i(\tau)\ \cdots\ \mathbf{a}_N(\tau)]\,,$$

$$B(\tau) \equiv \begin{bmatrix}\mathbf{a}^1(\tau)\\ \cdots\\ \mathbf{a}^j(\tau)\\ \cdots\\ \mathbf{a}^N(\tau)\end{bmatrix}, \quad \Delta\boldsymbol{\xi}(\tau) \equiv \begin{bmatrix}\Delta\xi^1(\tau)\\ \cdots\\ \Delta\xi^j(\tau)\\ \cdots\\ \Delta\xi^N(\tau)\end{bmatrix},$$

where

$$A(\tau)\,B(\tau) = B(\tau)\,A(\tau) = I,$$

I being the identity matrix, Note that by construction, the contribution $\Delta\mathbf{x}^e$ of the invariant subspace is identically zero.

A. The Framework Step-by-Step

The *G-Scheme* is fully described in [1]. Here the algorithmic steps of the framework are summarized with reference to Fig. 1. We use indices $i = 1,\ldots,N$, $a = H,\ldots,T$, $h = E+1,\ldots,H-1$, and $t = T+1,\ldots,N$.

We initialize the calculation by prescribing that $T(\mathbf{x}(t_0)) = N$, and compute $J(\mathbf{x}(t_0))$, $\lambda_i(t_0) = \lambda_i(\mathbf{x}(t_0))$, $A(t_0) = A(\mathbf{x}(t_0))$ and $B(t_0) = B(\mathbf{x}(t_0))$. Next, for each time interval t_n ($\tau = 0$), and for the state vector $\mathbf{x}(t_n)$, with $n = 0, 1, 2, \ldots$, we proceed as follows:

1) Define the time step as:

$$\Delta t = \gamma/|\lambda_{T(\mathbf{x}(t_n))}|, \qquad \gamma \le 1; \tag{1}$$

2) Update time:

$$t_{n+1} = t_n + \Delta t; \tag{2}$$

3) Find $H(\mathbf{x}(t_n))$ since, as discussed in [1], it depends on Δt;
4) Solve the set of non-stiff ODE's for $\tau \in \Omega = (0, \Delta t]$:

$$\frac{d\Delta\boldsymbol{\xi}^a}{d\tau} = B^a(t_n)\,\mathbf{f}\left(\mathbf{x}(t_n) + A_a(t_n)\,\Delta\boldsymbol{\xi}^a(\tau)\right), \qquad \Delta\boldsymbol{\xi}^a(0) = \mathbf{0}^a; \tag{3}$$

5) Update the state vector:

$$\mathbf{x}^a(t_{n+1}) = \mathbf{x}(t_n) + A_a(t_n)\,\Delta\boldsymbol{\xi}^a\,(\Delta t)\,; \tag{4}$$

6) Apply the head correction:

$$\mathbf{x}^h(t_{n+1}) = \mathbf{x}^a(t_{n+1}) + A_h(t_n)\,\Delta\boldsymbol{\xi}^h_{\mathrm{FF}}(\Delta t); \tag{5}$$

where the head correction is estimated as:

$$\Delta\boldsymbol{\xi}^h_{\mathrm{FF}}(\Delta t) = \Delta t\ B^h(t_n)\cdot \left[I + \frac{1}{2}\Lambda^h_h\left(\mathbf{x}(t_n), t_n\right)\Delta t\right]\mathbf{f}\left(\mathbf{x}(t_n)\right); \tag{6}$$

7) Apply the tail correction to project the solution onto the subspace obtained using the basis vectors found at t_n:

$$\mathbf{x}^t(t_{n+1}) = \mathbf{x}^h(t_{n+1}) + A_t(t_n)\,\Delta\boldsymbol{\xi}^t_{\mathrm{SIM}(t_n)}(\Delta t), \tag{7}$$

where the tail correction is estimated as:

$$\Delta\boldsymbol{\xi}^t_{\mathrm{SIM}(t_n)}(\Delta t) = -\left(B^t(t_n)J(\mathbf{x}(t_n))A_t(t_n)\right)^{-1}\cdot B^t\,(t_n)\,\mathbf{f}(\mathbf{x}^h(t_n)); \tag{8}$$

8) Update $J(\mathbf{x}^t(t_{n+1}))$, $\lambda_i(t_{n+1}) = \lambda_i(\mathbf{x}^t(t_{n+1}))$, and the set of new basis vectors $A(t_{n+1}) = A(\mathbf{x}^t(t_{n+1}))$ and $B(t_{n+1}) = B(\mathbf{x}^t(t_{n+1}))$;
9) Apply a bases rotation correction if necessary (*i.e.*, if the fast subspace changes) to find the state $\mathbf{x}(t_{n+1})$ by projecting $\mathbf{x}^t(t_{n+1})$ located on the manifold evaluated at t_n onto the manifold evaluated at t_{n+1}:

$$\mathbf{x}(t_{n+1}) = \mathbf{x}^t(t_{n+1}) + A(t_{n+1})\,\Delta\boldsymbol{\xi}_{\mathrm{SIM}(t_{n+1})}(\Delta t); \tag{9}$$

where the basis rotation correction is estimated as:

$$\Delta\boldsymbol{\xi}_{\mathrm{SIM}(t_{n+1})}(\Delta t) = -\left(B^t(t_{n+1})J(\mathbf{x}^t(t_{n+1}))A_t(t_{n+1})\right)^{-1}\cdot B^t\,(t_{n+1})\,\mathbf{f}(\mathbf{x}^t(t_{n+1})); \tag{10}$$

10) Find $T(\mathbf{x}(t_{n+1}))$ as discussed in [1];
11) Update the counter: $n = n + 1$;
12) If $[t_{n+1} < t_f]$ go back to step (1).

The choice of the safety factor γ has an impact on the local error of the solution, given that $\Delta t = \gamma\,O(\tau_T^p)$ where p is the formal order of accuracy of the quadrature scheme adopted to integrate (3).

IV. Results Using A Planar ODE Model

The reference solutions presented in this section are obtained with the module *NDSolve* in Mathematica© 6.0, the *Automatic* method of integration (by default an LSODA approach is used, switching between a non-stiff Adams method and a stiff Gear BDF method), a precision (or *rtol*) of 10^{-10}, and accuracy (or *atol*) of 10^{-14}. The calculations carried out with the *G-Scheme* use the explicit Runge-Kutta four-stage scheme (ERK4) to integrate the active dynamics, and, unless otherwise stated, we use $rtol = 10^{-4}$ and $atol = 10^{-13}$ in the threshold vector $\boldsymbol{\varepsilon}$ defined in [1]. We note that the present meanings of $rtol$ and $atol$ as used by *NDSolve* and the *G-Scheme* are somewhat different.

As a test featuring stiff explosive/dissipative nonlinear behavior, we use the Semenov model, which represents the dynamics of the first-order exothermal batch reaction $A \rightarrow B$ in a well-stirred jacketed reactor:

$$\frac{dy}{dt} = \varepsilon^{-1} f(y,z) \qquad \text{and} \qquad \frac{dz}{dt} = g(y,z),$$

where

$$f(y,z) = g(y,z) - \delta y \quad ; \quad g(y,z) = z \exp(y/(1+\beta y)),$$

with parameter values $\beta = 0.21$, $\delta = 1.0$, and $\varepsilon = 10^{-3}$, and initial condition $\{y(0), z(0)\} = \{5, 2\}$. The bifurcation properties of this model have been studied in [4]. This model problem is aimed at illustrating the operating characteristics of the *G-Scheme*.

For this set of parameters the solution proceeds from the initial condition to a fixed point (equilibrium), but with a fairly complex dynamics as can be seen from the phase trajectory or from the time evolution of y shown in Fig. 2. The relative error and the size of the time step are shown as functions of time in Fig. 3. The total number of time steps necessary to obtain the solution using the *G-Scheme* is 63. In Figs. 4 we show the number of active modes N_A, and the values of the head (H) and tail (T) indices as functions of time. It is clear from the figure that most of the time it is only necessary to integrate one ODE; integration of both ODEs is only necessary the first time step, and near the sharp corners shown in Fig. 2. We also see from Fig. 4 that from right after the initial condition until after the first turn $H = T = 2$. This indicates that the dynamics is effectively one-dimensional and is controlled by the fast time-scale (explosive stage). Afterwards, with the exception of the period spent in negotiating the second turn, the dynamics is again effectively one-dimensional, but this time it is controlled by the slow time scale (dissipative stage) since $H = T = 1$.

To illustrate the internal mechanics of the *G-Scheme*, Fig. 5 shows the contributions of the slow (head) and fast (tail) corrections to the phase trajectory. Note that in this two-dimensional Semenov model, as long as we have one active mode, then at any time only a head or tail correction to active dynamics can be applied. We see from the figure that in the first turn only head corrections are necessary. However, from the figure we see that small

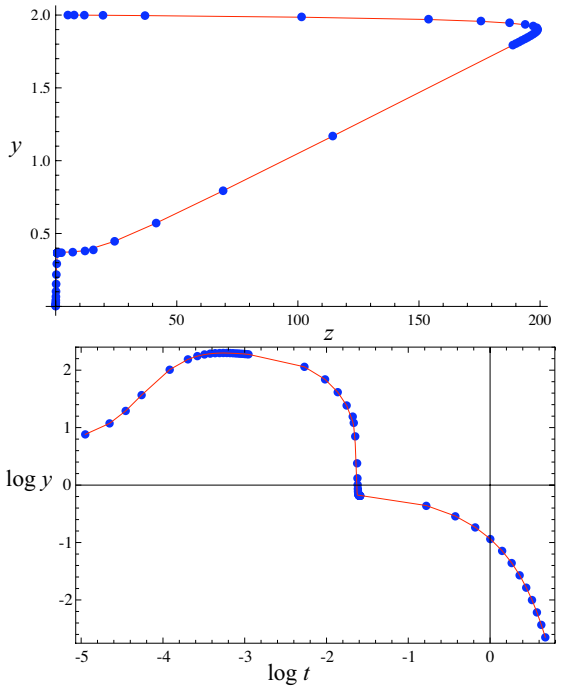

Fig. 2. Reference (line) and computed (points) trajectory in the (y, z)-plane and evolution of y.

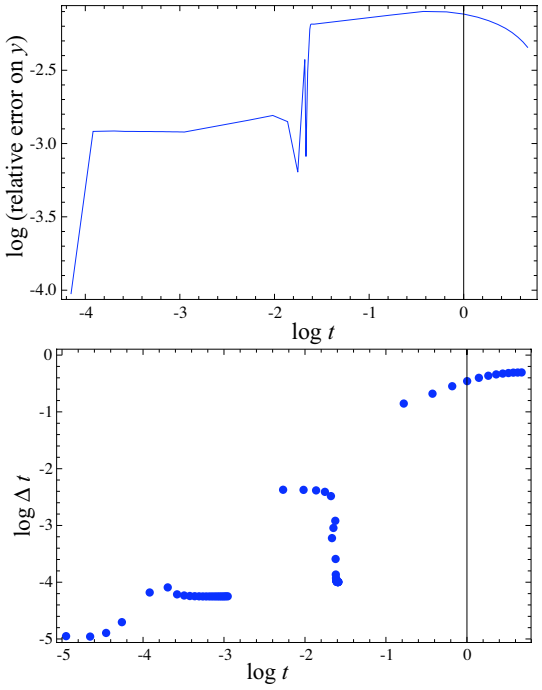

Fig. 3. Relative error on y and time step Δt as functions of time.

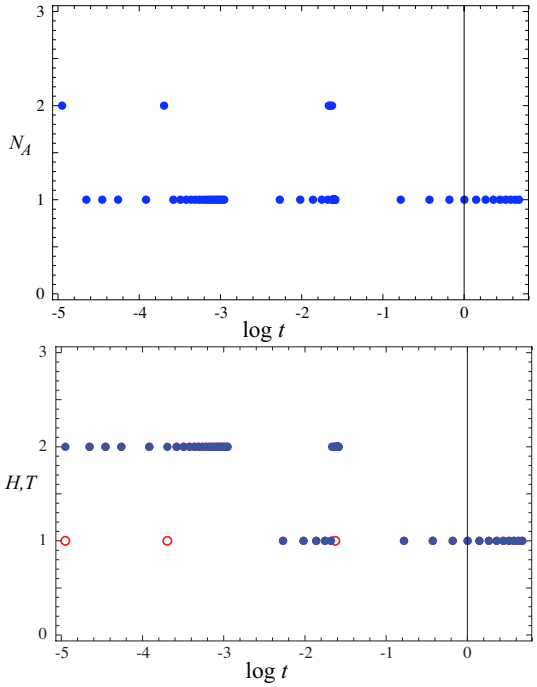

Fig. 4. Number of active modes N_A, and head H (hollow red circles) and tail T (solid blue circles) indices as functions of time.

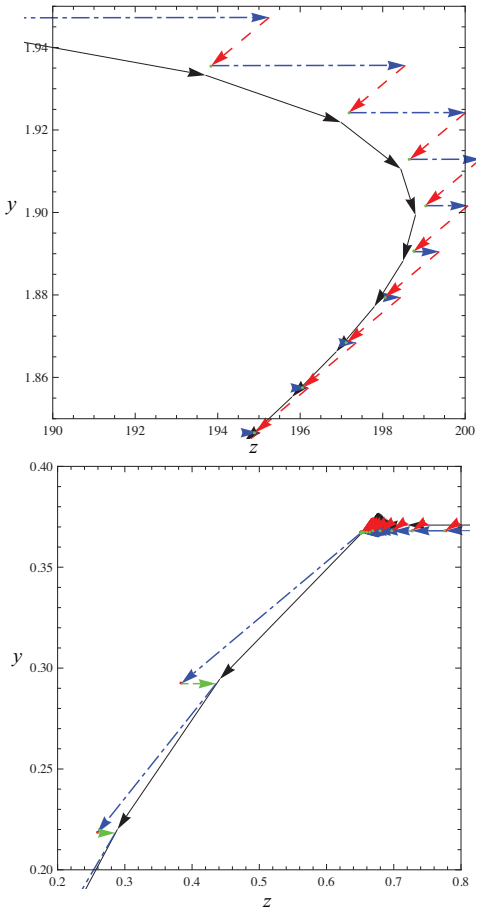

Fig. 5. Corrections to the state vector in the (y, z)-plane: reference (black line), active scales (short-long-dash blue line), head correction (long-dash red line), tail correction (short-dash green line).

head corrections are applied before the second turn, while tail corrections are necessary after the turn. In the figure, the blue arrows identify the state vector change due to the active time scales, the red/green arrows are parallel to the slow/fast direction and identify the state vector change due to the application of the head/tail correction, whereas the black arrows refer to the reference solution evaluated at the same time instants as the *G-Scheme* solution. The distance between the points of the red and black arrows or the green and black arrows is the error associated with the particular values of γ and $rtol$ used in this calculation.

V. Conclusion

We conclude by stressing that the main goal of this work is the presentation of the *G-Scheme* framework and the verification of its ability in achieving an adaptive model reduction. Regarding this aspect, the validation carried out by considering a range of test cases involving both linear and nonlinear behavior, both ODEs and PDEs, containing both simple and non trivial asymptotic dynamics, has successfully demonstrated the potential of the *G-Scheme* [1]. We already have successfully tested the *G-Scheme* in problems related to the kinetics of large hydrocarbons. In addition to addressing issues related to computational efficiency and error analysis, much work is still needed to translate this framework into a useful computational tool. We plan to make the package available to users and voluntary developers under the open-source paradigm in the near-future.

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References

[1] M.Valorani, S.Paolucci, The G-Scheme: A framework for multi-scale adaptive model reduction, In print, J.Comp.Phys. (2009).

[2] S.H.Lam, D.A.Goussis, The CSP method for simplifying kinetics, International Journal of Chemical Kinetics 26 (1994) 461–486.

[3] M.Valorani, D.A.Goussis, F.Creta, H.N.Najm, Higher order corrections in the approximation of low dimensional manifolds and the construction of simplified problems with the CSP method, J. Comput. Phys. 209 (2005) 754–786.

[4] F.Creta, A.Adrover, S.Cerbelli, M.Valorani, M.Giona, Slow manifold structure in explosive kinetics. 1. bifurcations of points-at-infinity in prototypical models, J. Phys. Chem. A 110(50) (2006) 13447–13462.