Equation-free, coarse-grained feedback linearization

Constantinos I. Siettos[1], Ioannis G. Kevrekidis[1,2] and Nikolaos Kazantzis[3]

Abstract— **We explore a systematic computational approach to the feedback regulator synthesis problem based on the "equation-free" timestepper methodology [2,3,4,5], where both the closed-loop dynamics linearization and pole-placement objectives are simultaneously attained in a single design step [1]. This is of particular interest in the case of systems/ processes modeled via microscopic/ stochastic simulations (e.g. kinetic Monte Carlo) for which coarse-grained, macroscopic models at the level we wish to control the behavior are not available in closed form.**

I. Introduction

An important assumption underlying the design of linear or nonlinear controllers for macroscopic problems is that explicit, reasonably accurate closed form dynamical models of the systems are available. Typically, such models arise in the form of conservation equations (mass, momentum, energy balances) closed through constitutive equations (e.g. the representation of viscous stresses for Newtonian fluids, or mass-action chemical kinetics expressions). However, in contemporary engineering problems, due to the stochastic/microscopic nature of the available models, and to nonlinear complexity, coarse-grained macroscopic equations are often not available in closed form. Instead, in many situations, the level at which the physics description may be available is a more detailed one: the evolution rules are known in the form of molecular dynamics, kinetic Monte Carlo, Markov-chain or hybrid schemes. In these circumstances, conventional continuum algorithms cannot be used explicitly for systems level analysis and controller design. Bridging systematically the enormous gap between microscopic space and time scales of a complex physical/material system and the macroscopic ones at which we want to design and control the behavior is a grand challenge for modeling and computation. Over the past few years we have demonstrated that "coarse timesteppers" [2,3,4,5,6,7], establish a link between traditional continuum numerical analysis and microscopic/ stochastic simulation. This is a mathematics assisted computational methodology, inspired from continuum numerical analysis, system identification and large scale iterative linear algebra, which enables microscopic-level codes to perform system-level analysis directly, without the need to pass through an intermediate, coarse-grained, macroscopic-level, "conventional" description of the system dynamics. The backbone of the method is the "on-demand" identification of the quantities required for continuum numerics (coarse residuals, the action of coarse slow Jacobians, eigenvalues, Hessians, etc). These are obtained by repeated, appropriately initialized calls to an existing time-stepping routine, which is treated as a black box. The coarse timestepper consists of the following elements (for a more detailed discussion see [2,3,4,5,6,7]:

(a) a lifting operator, transforming a macroscopic initial condition (typically zeroth- or first-order moments of the microscopically evolving distributions) to one (or more) consistent microscopic realizations,

(b) evolution of the microscopic realizations using the microscopic simulator for an appropriately chosen short macroscopic time T,

(c) a restriction operator, transforming the resulting microscopic distributions back to the macroscopic description

The key assumption is that deterministic, macroscopic, coarse models exist and close for the expected behavior of a few macroscopic system observables, yet they are unavailable in closed form. These observables (coarse-grained variables) are typically a few low moments of microscopically evolving distributions (e.g. surface coverages, the zeroth moments of agent distributions on

Manuscript received September 14, 2004. This work was partially supported by AFOSR and an NSF/ITR grant.

C. I. Siettos was with the Department of Chemical Engineering, Princeton University, Princeton, NJ, 08544, USA (e-mail: csiettos@Princeton.edu). Now he is with the School of Applied Mathematics and Physics, National Technical University of Athens, Greece.

I. G. Kevrekidis is with the Department of Chemical Engineering, Department of Mathematics and Program in Applied and Computational Mathematics, Princeton University, Princeton, NJ, 08544, USA (corresponding author, phone: (609) 2582818, e-mail: yannis@Princeton.edu).

N. Kazantzis is with the Department of Chemical Engineering, Worcester Polytechnic Institute, Worcester, MA, 01609-2280, USA (e-mail: nikolas@wpi.edu)

a lattice).

In this paper we attempt to solve the following problem: we assume that the model equations are not explicitly available, but we do have a black box subroutine (either a legacy timestepper, or a microscopic simulator) which, given the "macro"-state of the system $\boldsymbol{x} \in \mathrm{R}^n, u \in \mathrm{R}$ at time $t_k = kT$ reports the result of evolving the system after a time horizon T:

$$\boldsymbol{x}(k+1) = \boldsymbol{\Phi}_T(\boldsymbol{x}(k), u(k)) .$$

We develop a systematic approach to the feedback regulator synthesis problem based on the equation-free timestepper methodology where both the closed-loop dynamics feedback linearization and pole-placement objectives are simultaneously attained in a single design step [1] without being limited by the availability of an explicit dynamic model.

II. Nonlinear feedback linearization: background

One of the most popular controller synthesis methods involves the use of feedback in order to shape the dynamic characteristics of the controlled system, by appropriately placing the closed-loop poles at desirable locations on the complex plane (or equivalently, assigning the closed-loop dynamic modes or time constants). In the case of linear systems/processes, the synthesis of pole-placing state feedback control laws where the closed-loop eigenvalues (poles) are viewed as tunable parameters, has been very popular due to its intuitive appeal [9]. In the case of nonlinear systems, the traditional approach in designing pole-placing state feedback control laws is based on a local linearization of the system dynamics around a reference steady state, and the employment of linear design methods to attain the pole placement objective. This approach however, offers results of local validity that might lead to unacceptably poor performance of the controller, even in the presence of mild nonlinearities. In order to overcome the limitations that arise from the application of linear control methods to nonlinear systems, nonlinear feedback control laws need to be derived that are capable of directly coping with the process nonlinearities. In the pertinent body of literature, two main model-based pole-placing controller synthesis methods can be identified, that are both rooted in the area of geometric control theory [9]. The first one is the exact input/output (I/O) feedback linearization approach, where the introduction of nonlinear state feedback induces linear I/O behavior of the system of interest, by forcing the system's output to follow a pre-specified linear and stable trajectory [9].

This approach directly generalizes the linear result of placing the closed-loop poles at the system zeros and at a set of pre-specified values and is restricted within the class of minimum-phase systems. However, it should be pointed out, that regulation and/or stabilization of a system/process is understood in terms of forcing the system state to return to the design steady state (if driven away from it in the presence of disturbances) and not in terms of regulating a specific output at a given set point value (or output tracking).

The second approach is the geometric exact feedback linearization approach, realized by the following two-step design procedure [9]: as a first step, a simultaneous implementation of a nonlinear coordinate transformation and a state feedback control law is proposed, in order to transform the original nonlinear system to a linear and controllable one. The second step involves the employment of well-established linear pole-placement techniques for the transformed linear system. However, the geometric exact feedback linearization approach is based on a set of very restrictive conditions, that can hardly be met by any physical system [9].

III. Coarse timesteppers and feedback linearization with pole placement in one step: the approach

Consider the discrete time, autonomous nonlinear coarse system

$$\boldsymbol{x}(k+1) = \boldsymbol{\Phi}(\boldsymbol{x}(k), u(k)) , \ \Phi: \mathrm{R}^n \times \mathrm{R} \rightarrow \mathrm{R}^n \qquad (1)$$

where $x \in \mathrm{R}^n$ denotes the state vector, accessible through measurement, $u \in \mathrm{R}$ is the control variable and $\boldsymbol{\Phi}$ is a smooth function. Without loss of generality, it is assumed that $\boldsymbol{x=0}$ is the reference operating point (equilibrium point/coarse steady state) of (1), that corresponds to $u=0$, that is $\boldsymbol{\Phi}(\boldsymbol{0}, 0) = \boldsymbol{0}$.

The proposed methodology aims at simultaneously (in a single step) implementing a nonlinear coordinate transformation $\boldsymbol{z} = \boldsymbol{S}(\boldsymbol{x})$ coupled with a nonlinear state feedback control law $u = -\boldsymbol{cz} = -\boldsymbol{cS}(\boldsymbol{x})$, where $\boldsymbol{c}$ is an arbitrary constant row vector (a design parameter of the proposed method) that induce the desired linear closed-loop dynamics $\boldsymbol{z}(k+1) = \boldsymbol{A}\ \boldsymbol{z}(k)$ in the transformed variables. Notice, that $\boldsymbol{A}$ is the fundamental matrix of the closed-loop dynamics whose eigenvalues represent the inverses of the desirable closed-loop time-constants assigned by the proposed regulator, thus dictating the dynamic modes and speed under which regulation is performed. As shown in [1], the above design objective can be translated into a system of nonlinear functional equations (NFE's) that need to be satisfied by the unknown transformation map $\boldsymbol{S}(\boldsymbol{x})$:

$$\boldsymbol{S}(\boldsymbol{\Phi}(\boldsymbol{x}, -\boldsymbol{c}\,\boldsymbol{S}(\boldsymbol{x}))) = \boldsymbol{A}\,\boldsymbol{S}(\boldsymbol{x})$$
$$\boldsymbol{S}(\boldsymbol{0}) = \boldsymbol{0} \qquad (2)$$

The initial condition $\mathbf{S}(\boldsymbol{0}) = \boldsymbol{0}$ reflects the fact that equilibrium properties must be preserved under the

transformation. It can be shown [1] that the above system of NFE's admits a unique locally analytic and invertible solution $\boldsymbol{z} = \boldsymbol{S}(\boldsymbol{x})$ in a neighborhood of $\boldsymbol{x}=\boldsymbol{0}$. This single-step nonlinear regulator design approach allows us to circumvent the restrictive conditions associated with the first step of the classical exact feedback linearization method [9].

Remark 1: Notice that any fixed set-point tracking problem can be reformulated as a regulation problem such as the one under consideration.

Remark 2: The proposed feedback linearizing controller presupposes the availability of the full state vector for on-line measurements. The dual problem of designing an equation-free nonlinear observer that reliably reconstructs the unmeasurable states and induces linear error dynamics is feasible and currently being investigated by the authors.

From a practical point of view, the way to proceed when we have no explicit equations, is the following:

(a) Write the desired transformation vector $\boldsymbol{S}(\boldsymbol{x})$ as a power series expansion around the operating point of up to order p due to the underlying analyticity, i.e. write $\boldsymbol{S}(\boldsymbol{x})$ as $\boldsymbol{S}(\boldsymbol{x}; \boldsymbol{h})$, where $\boldsymbol{h} \in \mathrm{R}^n$ is the vector of the power series coefficients. For example for a 2-dimensional problem $\boldsymbol{S}(\boldsymbol{x}) \equiv \boldsymbol{S}(x_1, x_2)$ can be written as:

$$S_1(x_1, x_2; \mathrm{a_i}) = \mathrm{a}_1 x_1 + \mathrm{a}_2 x_2 + \frac{1}{2!}\mathrm{a}_3 x_1^2 + \frac{1}{2!}\mathrm{a}_4 x_2^2 + \mathrm{a}_5 x_1 x_2 + \ldots + \mathrm{O(p+1)}$$

$$S_2(x_1, x_2, \mathrm{b_i}) = \mathrm{b}_1 x_1 + \mathrm{b}_2 x_2 + \frac{1}{2!}\mathrm{b}_3 x_1^2 + \frac{1}{2!}\mathrm{b}_4 x_2^2 + \mathrm{b}_5 x_1 x_2 + \ldots + \mathrm{O(p+1)}$$

(b) Discretize the domain of the state-space in $N_1 \mathrm{x} N_2 \mathrm{x} \ldots N_n = N$ points (i.e. create a mesh of N points in the state-space where a numerical solution of the feedback linearization problem is sought).

(c) Calculate the values $\boldsymbol{h}$ of the unknown coefficients of $\boldsymbol{S}(\boldsymbol{x}; \boldsymbol{h})$ by solving the nonlinear least squares problem of the form:

$$\min_{\boldsymbol{x} \in R^n} \{\frac{1}{2}\sum_{i=1}^{N} \boldsymbol{G}_i(\boldsymbol{h})^2\},$$

$$\boldsymbol{G}_i(\boldsymbol{h}) = \boldsymbol{S}(\boldsymbol{\Phi}_{\mathrm{T}}(\boldsymbol{x}_i, -c\boldsymbol{S}(\boldsymbol{x}_i)); \boldsymbol{h}) - \boldsymbol{A}\boldsymbol{S}(\boldsymbol{x}_i; \boldsymbol{h}) \quad (3)$$

Quasi_Newton optimization methods as the Broyden, Fletcher, Goldfarb, Shamo (BFGS) method and/or a line search method (direct method) [8] can be used to minimize the above expression. The required (for the optimization code) values of $\boldsymbol{G}_i(\boldsymbol{h})$'s are evaluated through the timestepper for each point x_i in the mesh.

This nonlinear optimization problem can be solved in an iterative manner (by initially guessing a solution $\boldsymbol{h}_0$ and repeatedly calling the timestepper until convergence is attained).

It should be emphasized that microscopic simulators can be treated naturally in such a discrete time context, using the concept of the coarse timestepper. The one-step feedback linearizing controller is designed to stabilize the system's expected coarse behavior and assign the desirable set of time-constants to the controlled process, sidestepping the derivation of closed-form equations for this behavior (but assuming that such equations exist and close at the current level of description) [2,3,4,5,6,7].

IV. Simulation results: Applying coarse nonlinear feedback linearization to a kMC model

The proposed approach is evaluated through the use of a coarse time-stepper based on kinetic Monte Carlo models of simple surface reaction schemes for the simplification of the dynamics of NO oxidation by H_2 on Pt and Rh surfaces. The simplified deterministic mean field model is given by:

$$\frac{dx}{dt} = \alpha(1-x) - \gamma x - u(1-x)^2 x \quad (4)$$

where x is the coverage of adsorbed NO, α is a rate constant for NO adsorption, γ is the rate constant for NO desorption, and u is the reaction rate constant. Simulation results were obtained at: $\alpha = 1$, $\gamma = 0.01$; u is the bifurcation parameter (and, in our scheme, the control variable). Here we work with a kinetic Monte Carlo (stochastic) version of this heterogeneous catalytic reaction; for the stochastic simulations based on the mechanism whose mean field description is (4), the values of the number of available sites (system size), say $\mathrm{N_{size}}$, and $\mathrm{N_{run}}$, the number of realizations, were chosen here to be 100^2 and 100, respectively. At this point we should remind the reader that the Monte Carlo model is considered as a "black box" coarse timestepper $x(k+1) = \Phi(x(\mathrm{k}), u(\mathrm{k}))$. The time horizon was set to T=0.1s. The coarse Jacobian and the coarse eigenvalues are estimated by wrapping a computational superstructure like Newton's method as a shell around the coarse timestepper. The coarse identified model (Jacobian and right hand-sides) is then used for tracing the solution branch by coupling to a pseudo-arc-length condition. The corresponding coarse bifurcation diagram exhibits two regular turning points (at $u \approx 3.96$ and $u \approx 26$) (figure 1). What we want here is to derive a nonlinear feedback control law based on the above approach, to

stabilize the timestepper at the open-loop unstable stationary state (x_0 =0.5559, u_0 =4). To implement the above procedure and conform to the theory presented earlier we have used deviation variables defined as

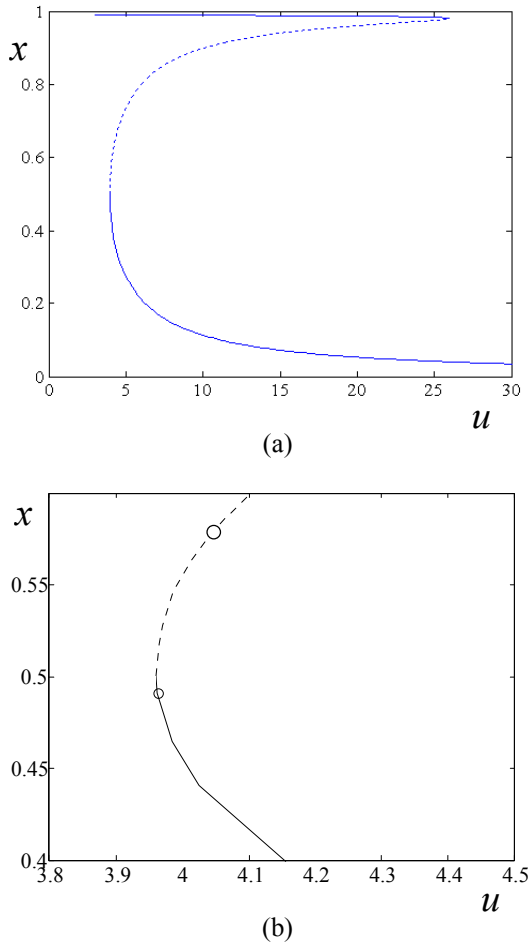

Fig. 1. (a) Bifurcation diagram of the kMC model, obtained by the coarse timestepper, (b) blow up of the diagram near the equilibrium of interest; solid lines correspond to stable steady states while the dotted ones correspond to unstable steady states.

$x' = x - x_0$ and $u = u - u_0$, while A now is a scalar chosen as 0.8 (a measure of the desirable speed of regulation). Here the variable x was discretized into 25 equally spaced points in [–0.1 0.1] and the unknown transformation $S(x)$ was derived numerically in the following two ways:

(a) analytically: by expanding S(x) in a second order power series of the form $S(x) = a_1 x + 0.5 a_2 x^2$ substituting $u = -S(x)$ into $\Phi(x(k), u(k))$ and then expanding the right hand side Φ in a 3rd order Taylor series around the equilibrium (0,0). The values of the unknown coefficients $a_{1,2}$ are then obtained by equating the series terms of the same order of both sides of NFE's (2).

(b) using the "black-box" timestepper approach: by solving the optimization problem as appearing in (3) for each timestepper.

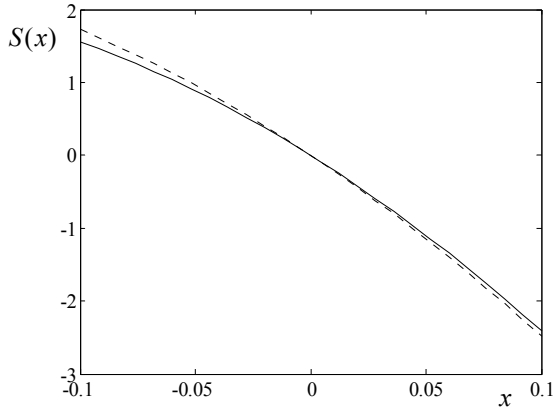

Fig. 2. S(x) as computed analytically (solid line) and using the proposed methodology using the black-box coarse KMC timestepper (dotted line).

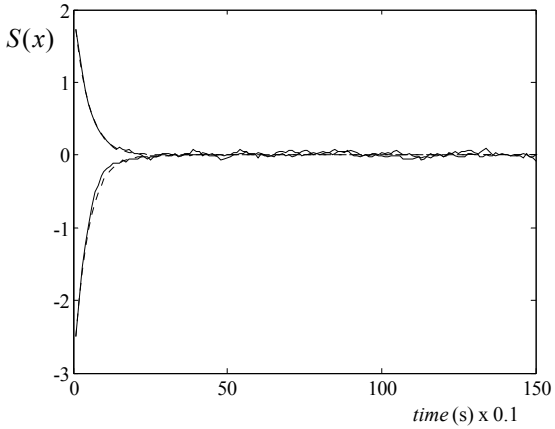

Fig. 3. Transients of $S(k+1)$=0.8 $S(k)$, corresponding to the desired closed loop dynamics, (solid lines) and S(x(k)) as obtained when applying the control law $u = -S(x)$ on the coarse KMC timestepper (dotted lines).

Figure 2 shows the computed $S(x)$ while figure 3 illustrates responses resulting from the desired closed loop dynamics $z(k+1) = S(k+1) = 0.8\ z(k) = 0.8\ S(k)$ (dotted lines) and that of the numerically obtained transformation $S(x)$ when applying the control law $u = -S(x)$ on the coarse timestepper (solid ones) .

Figure 4 shows the closed loop responses (after feedback linearization is attained through the approach described

above) of both the deterministic model and the kinetic Monte Carlo version of model (1) starting from different initial conditions. The feedback linearizing transformation was found by minimizing (2) using the BFGS method.

V. Conclusion

In the present study it was demonstrated that the performance of the proposed equation-free single-step feedback linearization method and the associated computational/algorithmic approach is quite satisfactory. Furthermore, this study represents a first promising research attempt suggesting that equation-free methods may play a useful role in designing coarse-grained nonlinear controllers for problems modeled by atomistic or stochastic simulators, and nanoscale systems in particular.

References

[1] N. Kazantzis,A functional equations approach to nonlinear discrete-time feedback stabilization through pole-placement, *Systems Control Lett.* , **43**, 361 (2001).

[2] K. Theodoropoulos Y.-H. Qian and I.G. Kevrekidis, Coarse stability and bifurcation analysis using timesteppers: a reaction diffusion example, *Proc. Natl. Acad. Sci*., **97**, 9840-9843 (2000).

[3] A. Makeev, D. Maroudas and I. G. Kevrekidis, Coarse statbility analysis using stochastic simulators: Kinetic Monte Carlo examples, *J. Chem. Phys.,* **116**, 10083-10091 (2002).

[4] I. G. Kevrekidis, C. W. Gear, J. M. Hyman, P. G. Kevrekidis, O. Runborg and K. Theodoropoulos, Equation-free coarse-grained multiscale computation: enabling microscopic simulators to perform system-level tasks, *Comm. Math. Sciences*, **1**, 715-762 (2003); original version can be obtained as physics/0209043 at arXiv.org.

[5] Siettos, C. I, Armaou, A., Makeev, A. G., Kevrekidis, I. G., Microscopic/ stochastic timesteppers and coarse control: a kinetic Monte Carlo example", *AIChE J*, **49**, 1922-1926 (2003).

[6] A. Armaou, C. I. Siettos and I. G. Kevrekidis, Time-steppers and coarse control of microscopic distributed processes, *Int. J. Robust and Nonlinear Control*, **14**, pp.89-111 (2004).

[7] I. G. Kevrekidis, C. William Gear and G. Hummer, Equation-free: the computer-assisted analysis of complex, multiscale systems, *AIChE J*, **50**, 1346-1354 (2004).

[8] C. T. Kelley, Iterative Methods for Optimization, SIAM series on Frontiers in Applied Mathematics, PA (1999).

[9] A. Isidori, Nonlinear Control Systems, Springer-Verlag,, New York (1999).

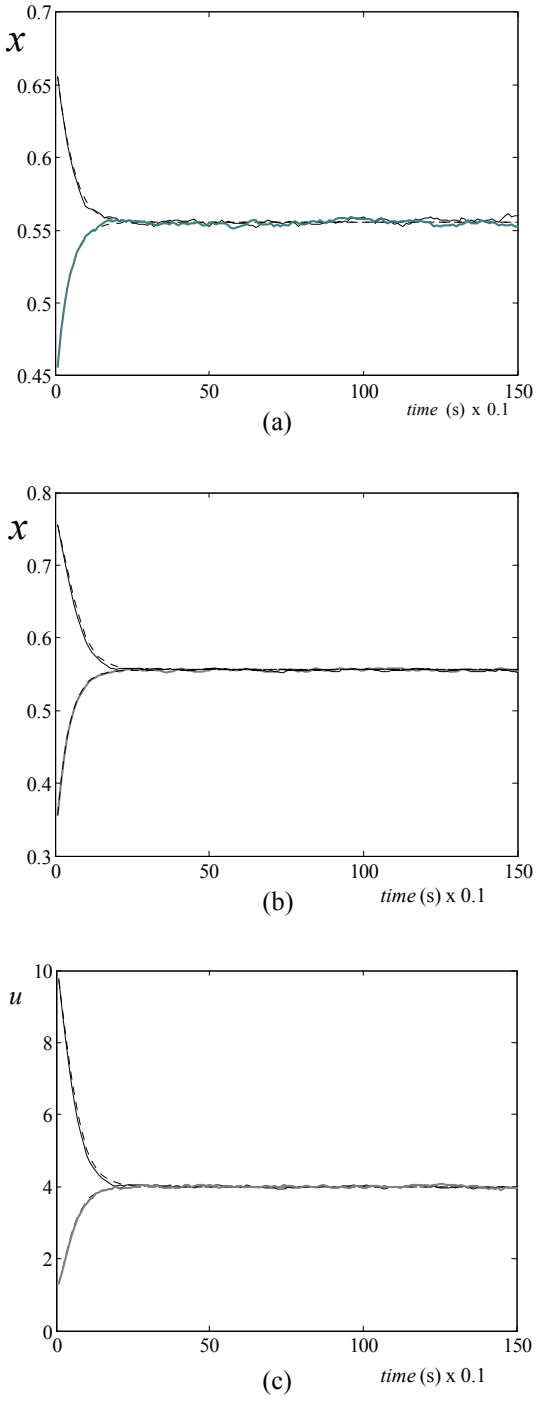

Fig. 4 (a) Transient response for $\pm$ 0.1 initial perturbation of the state variable from equilibrium. (b) Transient response for $\pm$ 0.2 initial perturbation of the state variable from equilibrium, (c) Transient response of the control variable for $\pm$ 0.2 initial perturbation of the state variable from equilibrium (lower ones correspond to –0.2 perturbation). Dotted lines correspond to the deterministic timestepper. Solid ones to kMC with Nsize=100and Nruns=10.