Detection of coarse-grained unstable states of microscopic/stochastic systems: a timestepper-based iterative protocol

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Received: 6 May 2010 / Accepted: 18 January 2011 / Published online: 12 February 2011
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Abstract We address an iterative procedure that can be used to detect coarse-grained hyperbolic unstable equilibria (saddle points) of microscopic simulators when no equations at the macroscopic level are available. The scheme is based on the concept of coarse timestepping (Kevrekidis et al. in Commun. Math. Sci. 1(4):715–762, 2003) incorporating an adaptive mechanism based on the chord method allowing the location of coarse-grained saddle points directly. Ultimately, it can be used in a consecutive manner to trace the coarse-grained open-loop saddle-node bifurcation diagrams of complex dynamical systems and large-scale systems of ordinary and/or partial differential equations. We illustrate the procedure through two indicative examples including (i) a kinetic Monte Carlo simulation (kMC) of simple surface catalytic reactions and (ii) a simple agent-based model, a financial caricature which is used to simulate the dynamics of buying and selling of a large population of interacting individuals in the presence of mimesis. Both models exhibit coarse-grained regular turning points which give rise to branches of saddle points.

Keywords Nonlinear dynamics · Bifurcation theory · Numerical detection of saddles · Large-scale systems · Complex systems · Coarse timestepping

1 Introduction

Many problems of current engineering, physical, and biological interest are characterized, due to the complexity of the underlying physics, by the lack of good macroscopic models in the form of ordinary, partial and/or integro-differential equations that can be used to describe the dynamic behavior in the continuum. When such continuum mathematical models are not available, microscopic simulations constitute the backbone of complex systems analysis practice. Several techniques ranging from kinetic Monte Carlo (kMC) to Molecular and Brownian Dynamics and from Cellular Automata to Individual and Agent-based simulations are being used extensively in many research areas as diverse as materials science [1–9], fluid mechanics [10–16], socioeconomic fields [17–21], neuroscience [22–29], epidemiology [30–34], ecology [35–37], biology [38, 39], car traffic, and pedestrian dynamics management [40–44].

However, due to the inherent stochasticity and the many-particles (atoms, molecules, macro-molecules, cells, tissues, individuals, populations) interactions, the emergent systems behavior at the macroscopic-continuum level is far from trivial to predict. Under this perspective, detailed simulations are used as
“computer experiments” in (a “loose”) analogy to the “physical experiments”: one sets up the (microscopic/experimental) initial conditions, the values of the parameters and performs runs (leaves the experiment to evolve) for long times (and for many microscopic ensembles consistent with the same initial conditions) in order to observe the macroscopic behavior. Yet, this is but the first thing one may employ in order to analyze the system’s coarse-grained dynamics. Important tasks such as the exact location of the critical points that mark the onset of instabilities cannot be easily obtained just through temporal simulations.

For the systematic and effective analysis of the simulation dynamics, one has to resort to bifurcation analysis. Numerical bifurcation theory provides an arsenal of algorithms and software packages \([45–50]\). While these are invaluable tools for performing systematic analysis for small to medium scale systems, there are some drawbacks in using them. On one hand, most of them require from the user to input the system evolution equations, which are assumed to be explicitly available in a specific way. One the other hand, linking them with legacy/commercial or “home-made” developed simulators is not something trivial. Furthermore, the convergence on unstable equilibria through such Newton-like solvers is most of the times impossible for microscopic/stochastic systems. In particular, for microscopic models, the lack of accurate macroscopic representations constitutes a major obstacle towards the systematic investigation of the systems behavior at the macroscopic level where the analysis is usually sought for design purposes.

Over the last years, it has been established that the so-called “Equation-Free” approach may efficiently confront with the problem in an integrated way \([51–60]\). This multiscale model reduction framework can be exploited to perform coarse-grained tasks such as bifurcation and stability analysis \([51, 53–55, 57–59, 61]\), controller design \([62, 63]\), computation of traveling waves, and periodic solutions \([64, 65]\), in a wide range of complex problems in mechanics and engineering, bypassing the need for extracting continuum-level equations in a closed form. The available detailed microscopic simulator is treated as a black-box timestepper of the coarse-grained observables; vital coarse-grained quantities, required for continuum numerical analysis (coarse residuals, the action of coarse Jacobians, control matrices, Hessians, etc.) and control design methodologies (linear, nonlinear, adaptive), are calculated on demand by using appropriately initialized short-in time-runs of the microscopic simulator. Based on this methodology, Siettos et al. \([66]\) present a dynamical feedback-based framework that enables microscopic/stochastic simulators to trace their coarse-grained bifurcation diagrams past turning points by coupling the concept of coarse timesteppers with wash-out filters and the so-called “linearized” pseudo-arc length condition. In \([67]\), Siettos et al. use an adaptive feedback control scheme to drive a microscopic simulator to its coarse critical point(s) and keep it there.

Many other efforts aspiring to bridge microscopic simulations, analysis and control design under a macroscopic model-based perspective have been proposed. Representative examples of this interplay include the construction of stochastic partial differential equations in order to design model predictive controllers (MPC) based on kMC simulations \([68–71]\), reduction-based techniques for Markovian systems \([72]\), stochastic parameter sensitivity analysis combined with multi-step optimization \([73]\) and the design of robust nonlinear feedforward-feedback controllers that dynamically couple kinetic Monte Carlo and finite difference simulation codes \([74]\).

In this paper, we address a new iterative procedure based on the concept of coarse-timestepping \([51, 53, 55, 56, 58, 59]\) that can be used to drive microscopic simulators—and potentially physical experiments—directly to their own open-loop unstable hyperbolic stationary points in a “vicinity” of a regular turning point. The approach does not require the implementation of a branch tracing method, such as the pseudo-arc length continuation, in order to reach the desired saddle point. If one wishes to trace the open loop codimension-one bifurcation branches of equilibrium she/he can do so in a consecutive manner, i.e., by implementing the approach for a fixed value of the bifurcation parameter and move on to the next one.

The paper is organized as follows: in Sect. 2, we present the proposed approach for the location of unstable fixed points (in particular saddles) using the coarse-timestepper-based iterative method. In Sect. 3, we demonstrate the scheme through two case studies: (a) a kinetic Monte Carlo simulation of a surface-reaction model and (b) an agent-based model approximating in a simplistic manner the dynamics of buying and selling of a large population of interacting individuals under the influence of mimesis. Finally, we conclude in Sect. 4.
2 Converging to a coarse-grained saddle: the procedure

2.1 The concept of the coarse-timestepper

Let’s assume that we do not have available the explicit macroscopic equations in a closed form, but we do have an evolving microscopic (or a very-large scale) computational model. Given the (microscopic) distribution of the system \( U_k = U(t_k) \in \mathbb{R}^N \), \( N \gg 1 \) at time \( t_k = kT \), the detailed simulator reports the values of the state variables after a time interval \( T \), i.e.,

\[
U_{k+1} = \varphi_T(U_k, p),
\]

where \( \varphi_T : \mathbb{R}^N \times \mathbb{R}^m \rightarrow \mathbb{R}^N \) is the time-evolution operator, \( p \in \mathbb{R}^m \) is the vector of systems parameters.

The main assumption behind the coarse timestepper is that a coarse-grained model for the fine-scale dynamics (1) exists and closes in terms of a few coarse-grained variables, say, \( x = [x_1, x_2, \ldots, x_n] \in \mathbb{R}^n \), \( n \ll N \).

Usually, these are the low-order moments of the microscopically evolving distributions. The existence of a coarse-grained model implies that the higher order moments, say, \( y \in \mathbb{R}^{N-n} \), of the distribution \( U \) become, relatively fast over the coarse time scales of interest, functions of the few lower ones, \( x \). This scale separation can be viewed in the form of a singularly perturbed system of differential equations:

\[
\begin{align*}
\frac{dx(t)}{dt} &= f(x, y, p), \quad x(t = 0) = x_0, \quad (2a) \\
\epsilon \frac{dy(t)}{dt} &= g(x, y, p), \quad y(t = 0) = y_0 \quad (2b)
\end{align*}
\]

where \( \epsilon \) is a small positive parameter, i.e. \( \epsilon \ll 1 \). Equation (2a) corresponds to the “slow” coarse-grained dynamics while (2b) to the “fast” ones. Assuming that both \( x(t) \) and \( y(t) \) are differentiable, the above system of equations can be written, in a discrete time representation as:

\[
\begin{align*}
x_{k+1} &= h_s(x_k, y_k, p), \quad (3a) \\
\epsilon y_{k+1} &= h_f(x_k, y_k, p). \quad (3b)
\end{align*}
\]

where

\[
h_s(\cdot) = x_k + \int_{t_0}^t f(s, x(s), y(s)) \, ds
\]

\[
h_f(\cdot) = \epsilon y_k + \int_{t_0}^t g(s, x(s), y(s)) \, ds
\]

Fig. 1 The basic assumption of the equation-free approach: the higher order moments \( y \) of an evolving microscopic distribution become “quickly”—within the time-horizon \( T \)—functionals of the lower-order moments \( x \)

Notice that under certain conditions [75] the overall dynamics defined by (3) will approximate very quickly the dynamics of the following system:

\[
\begin{align*}
x_{k+1} &= h_s(x_k, y_k, p), \quad (4a) \\
0 &= h_f(x_k, y_k, p). \quad (4b)
\end{align*}
\]

The system above can—under some mild assumptions [75] be written in the form of

\[
x_{k+1} = F(x_k, p). \quad (5)
\]

This is achieved by applying the implicit function theorem for (4b), giving:

\[
\begin{align*}
y_k &= q(x_k), \quad (6a) \\
F(x_k, p) &\equiv h_s(x_k, q(x_k, p), p). \quad (6b)
\end{align*}
\]

where \( q \) is a smooth continuous function defining the relation between the slow and the fast variables after a short (in the macroscopic sense) time horizon. Equation (6a) constitutes the slow manifold on which the coarse-grained dynamics of the system evolve after a fast transient phase (see Fig. 1).

What a coarse timestepper does, in fact, is providing such closures on demand: relatively short calls of the fine scale simulation can establish this “slaving” relation (refer to [51, 53, 55, 56, 58, 59] for...
more detailed discussions). Briefly, once the appropriate macroscopic observables have been identified, the coarse timestepper consists of the following essential components (Fig. 2):

(a) Prescribe the coarse-grained initial conditions (e.g., the distribution of the temperature and concentration of the species in a combustor, the distribution of positions and velocities in a Molecular Dynamics box, etc.) \( x(t_0) \equiv x_0 \).

(b) Transform it through a lifting operator \( \mu \) to consistent microscopic realizations:

\[
U(t_0) = \mu x(t_0)
\]

(c) Evolve these realizations in time using the microscopic simulator for a short macroscopic time \( T \) generating \( U(t_0 + T) \). The choice of \( T \) is associated with the (estimated) spectral gap of the linearization of the unavailable closed macroscopic equations [53, 60].

(d) Obtain the coarse-grained variables using a restriction operator \( M \):

\[
x_{k+1} \equiv x(t_0 + T) = M U(t_0 + T)
\]

2.2 Description of the iterative scheme

Starting from a stable equilibrium (a node), \( (x^*_n, p^*_i) \), where \( x^*_n = F(x^*_n, p^*_i) \), the objective is to drive the detailed large-scale simulator to its own coarse-grained saddle point(s) (if any) at a prescribed value of the bifurcation parameter, say \( p^*_i \), which is assumed to be “relatively close” (we explain this term below) to the turning point, say \( p^{critical}_i \). We also assume that both the starting stable node and the (unknown) saddle are lying on solution branches connected through a saddle-node bifurcation at \( p^{critical}_i \).

Given \( p^*_i \), our procedure drives the system to the objective by creating a sequence of actions

\[
 u_{seq} = \{u_1, u_2, \ldots, u_j, \ldots, u_n\},
\]

where

\[
u_j \equiv \Delta p_j = p^i_j - p^*_i
\]

and \( p^i_j \) is the appropriately computed value of \( p_i \) at step \( j \).

The sequence should converge to zero for deterministic systems (or within a small tolerance, \( tol_1 \), that can be defined with respect to the system’s relative noise for stochastic/microscopic systems), i.e.

\[
u_n \approx 0.
\]

Hence, upon convergence we have that

\[
p^i_j \approx p^{*}_i.
\]

In a “vicinity” of the regular turning point the systems dynamics (5) close to equilibria are characterized by a separation of time scales and the emergence of a one-dimensional slow manifold. Hence, the trajectories \( x(t) \) can be decomposed into fast \( \eta(t) \) and slow \( w(t) \) ones, whose dynamics can be represented as a singularly perturbed system of the form

\[
\eta_{k+1} = s(\eta_k, w_k, p), \quad \eta \in \mathbb{R},
\]

\[
\varepsilon w_{k+1} = f(\eta_k, w_k, p), \quad w \in \mathbb{R}^{n-1}.
\]

The value of \( \varepsilon \) gets smaller as the separation between the coarse-grained time-scales gets wider. After an initial time interval \( t > T_r \) and under the assumptions of the Fenichel theorem [75] the dynamics of the above system can be approximated by the reduced slow system

\[
\eta_{k+1} = s(\eta_k, \phi(z_k), p),
\]

where \( \phi \) is a sufficiently differentiable function of \( \eta \), relating the fast \( w \), and slow \( \eta \), coarse grained variables as

\[
w = \phi(\eta).
\]

The above \((n-1)\) scalar equations define a curve which forms the one-dimensional slow manifold. In a neighborhood of a saddle point \((x^s, p_i)\), this is tangent to the linear unstable manifold spanned by the
eigenvector $e_u$ corresponding to the dominant unstable eigenvalue $\lambda_u$ ($|\lambda_u| > 1$) of the Jacobian of the linearized system:

$$\delta x_{k+1} = \frac{\partial F}{\partial x} \delta x_k,$$

where $\delta x_k = x_k - x^s$ and $\frac{\partial F}{\partial x}$ is the Jacobian evaluated at $x^s$.

Let us now denote the open ball in $R^n$ with radius $\varepsilon$ and center $x$ defined by

$$B(\varepsilon, x) = \{ z : \| x - z \| < \varepsilon \}.$$

In a sufficiently small neighborhood of a saddle point $(x^s, p_i) : x^s = F(x^s, p_i),$ and after some time horizon, $\forall z \in B(\varepsilon, x^s),$ excluding the points defining the coarse-grained separatrix, $\exists \delta(\varepsilon)$:

$$\| F(z, p_i) - z \| > \delta(\varepsilon).$$

Equation (13) implies that sufficiently close to the saddle point the system’s dynamics will—within a certain relatively small time horizon—evolve monotonically away from the saddle, i.e.,

$$\| x_{k+1} - x^s \| > \| x_k - x^s \|,$$

along the (linear) one-dimensional coarse-grained unstable slow manifold. If the gap between the coarse-grained time scales in (8) is big enough, the dynamics will eventually approach very fast, and then evolve along, the “slow” eigenvector, i.e.,

$$\delta x_{k+1} \rightarrow c_u \lambda_u e_u,$$

where the coefficient $c_u \in R$ is associated with the initial conditions. Starting from a nearby initial point at the “other side” of the separatrix, the dynamics will eventually evolve along the opposite direction, i.e.,

$$\delta x_{k+1} \rightarrow c_u \lambda_u (-e_u).$$

This behavior is justified by the Hartman–Grobman theorem stating that in the vicinity of hyperbolic points the local nonlinear dynamics are topologically equivalent with the linear ones [76].

In summarizing, starting from a detailed initial distribution, the system will quickly approach the “slow” coarse-grained manifold as defined by (6a) and then move along the unstable coarse-grained manifold as defined by (10); in the neighborhood of an equilibrium point and under the above assumptions, the coarse-grained dynamics will evolve along $e_u$, i.e., along the eigenvector corresponding to the dominant eigenvalue of the linearized problem (11) (see Fig. 3).

Depending on the initial conditions $x_0$ across the coarse-grained separatrix, the system will ultimately approach the stable fixed point $x_n$ or move toward another attractor, say $A$ (such as another stable fixed point).

Due to continuity, for small perturbations of the control parameter, i.e., for $u_{j+1} = u_j + \delta u$, the direction of the dominant eigenvector as well as the value of the corresponding eigenvalue and generally the behavior of the trajectories do not change considerably, i.e., they remain qualitatively unchanged. Hence, by monitoring an observable such as the difference $(x^k_{k+1} - x^k_i)$ with the maximum norm—we can infer about the side of the separatrix that the coarse grained dynamics evolve.

Under the above assumptions, our algorithm reads as follows:

**Step 0.** Initialize the sequence with $u_0 > 0$ or $u_0 < 0$ if $p_i^l < p_i^{\text{critical}}$ and $p_i^r > p_i^{\text{critical}}$, respectively. A loose estimate of the value of $p_i^{\text{critical}}$ can be obtained by plain temporal simulations.

As we consider the parameters’ values of the vector $\{ p - \{ p_i \} \}$ as constants, we rewrite the coarse timestepper model on the slow manifold as

$$x_{k+1} = F(x_k, p_i^k).$$

**Step I.** Initialize the algorithm with the required parameters: gain, tol, tol', c, tol2.
All parameters of the iterative protocol may be in principle constants or can be changed adaptively. Set $k = 1$ and go to Step II.

**Step II. Do While convergence to the saddle point** (i.e. when $|u_k| < tol_1$)

A. We “perturb” the system for a macroscopic time horizon $T$ using $u_{k-1}$ as our “control” action to get

$$U_k = \varphi_T(U_{k-1}, p^{k-1}).$$  \hspace{1cm} (17)

B. Set the initial interval of the possible values of $u_k$ as follows:

If $u_{k-1} > 0$ Then

set interval $= [lB_0, uB_0] = [0, u_{k-1}]$;

Else

set interval $= [lB_0, uB_0] = [u_{k-1}, 0]$;

Endif

Set $q = 0$;

C. *Do while* $|h(d)| > tol_2$ (see below, how $h(d)$ is defined) using a Chord-like technique

1. Update $q = q + 1$; compute the next “control” action from

$$u_k = lB_{q-1} + a(uB_{q-1} - lB_{q-1}),$$  \hspace{1cm} (18)

where $0 < a < 1$.

2. Compute the coarse-grained state vector by letting the detailed simulator to relax on the coarse-grained slow manifold corresponding to the new value of $u_k$. This can be achieved by running the detailed model for a sufficiently small time horizon $T_r$:

$$U_{k+1} = \varphi_{T_r}(U_k, p_i^k).$$  \hspace{1cm} (19)

Upon the coarse-grained slow manifold, monitor the evolution of the dynamics for a short time $T_s$:

$$x_t = F_{T_s}(x_0, p_i^k),$$  \hspace{1cm} (20)

where $x_0$ is the coarse-grained state vector as obtained by restricting $U_{k+1}$.

3. Calculate the function $h : R^n \rightarrow R$ reading

$$h(x_t) = x_t^i - x_0^i, \hspace{0.5cm} |x_t^i - x_0^i| := \max_{j=1}^p(|x_t^j - x_0^j|).$$  \hspace{1cm} (21)

4. Update the search space of $u_k$ according to the following manner:

a. If $h(d) < 0$ (meaning—under our convention—that the coarse-grained fixed point of (20) is located at $p_i^k > p_i^* + u_k$) Then set $lB_q = u_k$;

Else If $h(d) > 0$ (meaning that the equilibrium is located at $p_i^k < p_i^* + u_k$) Then set $uB_q = u_k$;

Endif

b. If $(uB_0 == lB_q$ or $lB_0 == lB_q$ and $uB_q - lB_q < tol_2$; i.e., the procedure has minimized the search space to some extent and the control action cannot drive the system from one region of attraction to the other Then

If $uB_0 == lB_q$; Then update the bounds of the control action as

$$uB_0 = uB_0 + c, uB = uB_0;$$

Else

$$lB_0 = lB_0 - c, lB = lB_0;$$

Endif

Endif

In summary, the above iterative procedure converges to the fixed point of the map $x = F(x, p_i^k)$ (and as a consequence it minimizes $|h(d)|$) by manipulating $p_i^k$ (see also Fig. 4).

**End Do While (of Step II. C)**

D. Update $k = k + 1$ and run the detailed model for a time horizon $T_r : U_k = \varphi_{T_r}(U_{k-1}, p_i^{k-1})$ in order to relax the system to the slow manifold.

E. Update the new action as

$$u_k = \text{gain} \cdot u_{k-1}.$$  \hspace{1cm} (22)

The value of the gain should be greater than one in order to drive the system (applying the control action as defined by (18)) closer to the seeking saddle point (see Fig. 4). Its value could be constant or adaptively depending on how far is the current control action $p_i^k$ from the nominal value $p_i^*$. If the system is currently at the coarse-grained saddle point, $u_{k-1} = 0$, the next action will be also $u_k = 0$.

Set $k = k + 1$.

**End Do While (of Step II)**

The procedure finds the intermediate “control/iterative” actions through the chord method in order to “traverse” in some way the turning point and drive the system to the saddle point that we are seeking.
A feature of the method is that it does not require the reconstruction—through lifting—of consistent high-dimensional microscopic/detailed distributions from the low-dimensional coarse-observables. What is fed into the algorithm is a “snapshot” of the microscopic distribution ($U_k$ in (19)) whose projection $x_0$ into the low-dimensional space serves as the initial guess into the chord-like iteration [77].

Under our assumptions, the steering of the system toward the coarse-grained saddle is achieved by manipulating the “control” parameter by-passing the necessity for using a conventional Newton–Chord-like technique [77]. Hence, it does not require the numerical approximation of the system’s coarse-grained Jacobian $\nabla F(x_k)$, which would (a) increase the computational cost requiring the computation of all first-order partial derivatives of the vector field $F(\cdot)$, (b) require the derivation of consistent to the coarse-grained variables detailed/microscopic distributions. For stochastic systems, Step II.C.2 should be repeated for a number of ensembles and then take the average of the results.

To this end, we should note that the proposed methodology does not infer about the system’s stability in an explicit manner, as it does not calculate the eigenvalues of the Jacobian. For large-scale systems, stability analysis can be performed, upon convergence, by wrapping around the timestepper an iterative eigen-solver such as Arnoldi procedure. For low-scale systems, the stability analysis can be performed by calculating the eigenvalues of the “small-size” Jacobian. The numerical approximation of the Jacobian is possible, upon convergence, by calling the timestepper, at appropriately perturbed values of the corresponding coarse-grained variables.

3 Case studies and simulation results

We demonstrate our method using two case studies. The first one is a kinetic Monte Carlo (kMC) realization of a chemical reaction on a catalytic surface while the second one is a simplistic agent-based model of buying and selling dynamics under the influence of mimesis which bears strong analogies to integrate-and-fire models of neurons.

3.1 Kinetic Monte Carlo simulations of surface reactions

We first present an example describing the dynamics of simple catalytic reactions using stochastic simulations. The species react, are adsorbed or desorbed on
a finite lattice with periodic boundary conditions. At each time instant, the sites of the lattice are considered to be either vacant or occupied by the reaction species. In the kMC context, the system’s dynamics are described by the following chemical master equation:

\[
\frac{dP(x,t)}{dt} = \sum_{y \neq x} Q(x,y) P(y,t) - \sum_y Q(x,y) P(x,t),
\]

(23)

where \(P(x,t)\) is the probability that the system will be in state \(x\) at time \(t\). \(Q(x,y)\) denotes the probability for transition from state \(y\) to \(x\) per unit time. The summation runs over all possible transitions (reactions), say, \(N_r\).

Here, we used the Gillespie kMC algorithm [78, 79] to numerically simulate the above stochastic equation. The basic steps read as follows:

**Do While** \{time < \text{end}\}

1. Calculate the cumulative transition probability \(Q_0(N_r) = \sum_{y=1}^{N_r} Q(x,y)\).
2. Draw two random numbers, say \(r_1\) and \(r_2\), from a uniform distribution in the interval [0, 1].
3. Select the reaction \(y^*\) from the set of all possible events so that the following inequality is satisfied:

\[
Q_0(y^* - 1) < r_1 Q_0(N_r) < Q_0(y^*).
\]

(24)

4. Perform the selected event and update all kinetic rates according to the occurred event.

5. Advance time by \(\Delta t = -\frac{1}{Q_0(N_r)} \ln r_2\), \text{time} = \text{time} + \Delta T\)

**End DoWhile**

Our illustrative microscopic model is a kMC realization of a simplification of the dynamics of catalytic CO oxidation:

\[
\text{CO} + \frac{1}{2} \text{O}_2 \rightarrow \text{CO}_2.
\]

(25)

The reaction mechanism can be schematically described by the following elementary steps:

1. \(\text{CO}_{\text{gas}} + *_i \leftrightarrow \text{CO}_{\text{ads},i}\),
2. \(\text{O}_2,\text{gas} + *_i + *_j \leftrightarrow \text{O}_{\text{ads},i} + \text{O}_{\text{ads},j}\),
3. \(\text{CO}_{\text{ads},i} + \text{O}_{\text{ads},j} \rightarrow \text{CO}_{\text{gas}} + *_i + *_j\),

(26)

where \(i, j\) are sites on the square lattice, * denotes a site with a vacant adsorption site, while “ads” denotes adsorbed particles. A simple schematic of the above mechanism is given in Fig. 5.

The macroscopic mean field description is given by the following equations [61]:

\[
\dot{\theta}_A = \alpha (1 - \theta_A - \theta_B) - \gamma \theta_A - 4k_r \theta_A \theta_B,
\]

(27a)

\[
\dot{\theta}_B = 2\beta (1 - \theta_A - \theta_B)^2 - 4k_r \theta_A \theta_B,
\]

(27b)

where \(\theta_l\) represent the coverage of species \((l = A, B, \text{corresponding to CO and O})\) on the catalytic surface. The parameters \(a, \beta, \gamma\) are associated with CO adsorption, O dissociative adsorption, and CO desorption rates while \(k_r\) is a reaction rate constant. The asymmetric inhibition of CO and O oxidation introduced in (26): CO can adsorb on an O-covered surface and not vice versa follows from experimental observations [80–83].

Here, the system’s size and the number of realizations were chosen to be \(N_{\text{size}} = 1000 \times 1000\) and \(N_{\text{runs}} = 2000\), respectively. The value of the time horizon was selected as \(T = 0.05\).

The coarse timestepper

\[
\theta_{A,k+1} = \Phi_{1,T}(\theta_A, \theta_B, \beta, a, k_r),
\]

(28a)

\[
\theta_{B,k+1} = \Phi_{2,T}(\theta_A, \theta_B, \beta, a, k_r)
\]

(28b)

of the kMC realization was used as a “black box” timestepper.

Figure 6a depicts the convergence of the coarse-grained variables for \(a = 1.6, \beta = 4, \gamma = 0.04, k_r = 1\), to the correct value of the saddle point at \(\theta^*_A = 0.7323, \theta^*_B = 0.0881\) starting from either \(\theta^*_A = 0.9701, \theta^*_B = 0.0016\), or \(\theta^*_A = 0.1126, \theta^*_B = 0.6902\) stable equilibria; Fig. 6b depicts the corresponding “control” action sequence of the parameter \(a\).
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By repeated calls of the procedure for different values of the parameter $\beta$, we also calculated the corresponding coarse-grained bifurcation diagram with respect to $\beta$ (shown in Fig. 7). The obtained diagram coincides with the one obtained through the deterministic system (22) (see also [61]). The inset in Fig. 7 depicts the sequence of the algorithm as seen on the 1-D bifurcation diagram using $\beta$ as “control” action.

To this end, Fig. 8 depicts the diagram of the two eigenvalues of the Jacobian of the deterministic mean field model (27) at the fixed points. The “slow” eigenvalue changes sign at the turning points. There is a clear separation in time scales.

3.2 Agent-based simulation of a financial market caricature

Our second illustrative example is an agent-based model describing a simplistic buyer-seller procedure appearing in [84]. Consider a market with $N$ individuals. The state $x_i$ of each individual $i = 1, 2, \ldots, N$ is a scalar in the interval $(-1, 1)$. The value of $x_i$ reflects the “mood” of agent $i$ to buy or sell. At $-1$ individuals
sell, at +1 they buy; then their mood is reset to neutral (zero). Thus, the main activity is the evolution of the state \( x_i \) of the individuals within \((-1, 1)\); this is modeled by the following stochastic differential equation:

\[
\frac{dx_i(t)}{dt} = -\gamma x_i(t) + I_i(t) \tag{29}
\]

coupled with the constraint that when the state reaches the thresholds \(-1, 1\) it is immediately reset to \( x_i = 0 \). \( I_i(t) \) is a stochastic variable representing the incoming information arriving to the individual \( i \) at time \( t \). This can be considered as the exogenous information each individual draws from its environment (e.g., mass media news, or opinions of stock market consultants) plus the influence due to recent decisions of other agents. Each agent reacts to such “good” or “bad” news and its state, \( x_i \), is increased by \( \varepsilon^+ \) or decreased by \( \varepsilon^- \), respectively. The arrival of the news comes at discrete times with Poisson distributed rates of \( \nu^+_{ex} \) and \( \nu^-_{ex} \), respectively. Hence, the state of each agent changes in an event-driven way by a series of positive or negative jumps at times \( t^{(k)}, k = 1, 2, 3, \ldots \). In the absence of such stimuli, the state of each individual is exponentially attracted to zero (no particular interest to buy or sell) at rate \( \gamma \). Agents are also influenced by the overall buying and selling rates. When one agent buys (sells) the probability of all other agents, buying (selling) increases for a short period of time. We model this by computing a buy (sell) rate over an interval \( \Delta t \) as

\[
R^\pm = \frac{number \, buys \, (sells) \, in \, (t, t + \Delta t)}{\Delta t} \tag{30}
\]

and then increasing the rate of incoming information per agent to

\[
v^\pm = v^\pm_{ex} + g R^\pm \tag{31}
\]

g is a factor representing the relative influence of the buying and selling rates. When \( g \ll N \), then the inputs to the agents can be considered for practical reasons as uncorrelated.

For the numerical integration of (1), the choice here is an explicit Euler method resulting to

\[
x_i(t + dt) = (1 - \gamma \delta t)x_i(t) + dt I_i(t). \tag{32}
\]

In that case, the buying and selling rates per agent can be approximated by

\[
R^\pm = \frac{1}{N \delta t} \sum_{i=1}^{N} \delta(n - i), \tag{33}
\]

where \( n \) denotes the agent who crosses \(-1\) or \( 1 \) between time \( t \) and \( t + \delta t \).

For our simulations, we used the following values for the parameters: \( v^+_{ex} = 20, v^-_{ex} = 20, \nu^+_{ex} = 20, v^-_{ex} = 20, \varepsilon^+ = 0.075, \varepsilon^- = 0.075, \gamma = 1, \delta t = 0.25 \). The number of agents of the system was set to \( N = 50000 \); the observable of our method is the average state \( \bar{x} = \frac{1}{N} \sum_{i=1}^{N} x_i \).

Figure 9 depicts the coarse-grained bifurcation diagrams of \( \bar{x} \) vs. \( v^\pm_{ex} \) as constructed by repetitive calls of the proposed procedure for \( g = 38 \), while Fig. 10
Fig. 10 The coarse-grained bifurcation diagram of the agent-based model, with $g$ serving as the bifurcation parameter. It was obtained by implementing the proposed iterative protocol for consequent values of $g$.

shows the coarse-grained bifurcation diagram $\bar{x}$ with respect to the parameter $g$ as this obtained by implementing the protocol in an iterative way for consecutive values of $g$. Figures 11a, b show the convergence of $\bar{x}$ and the computed “control-iterative” actions required to drive the system at the upper coarse-grained saddle stationary point for $g = 38$, using $v_{\text{ex}}^+$ as the “control” parameter. Figures 11c, d illustrate the convergence of $\bar{x}$ to the lower saddle point and the “control” actions sequence, respectively, using $v_{\text{ex}}^-$ as the “control” parameter.

4 Conclusions

Microscopic simulation is a vital tool in the study of complex and multiscale phenomena ranging from Material Science and Mechanics to Engineering, Ecology, Biology, and Social Sciences.

We introduced and demonstrated a new iterative procedure based on the concept of coarse-timestepping [53] that can be used to drive microscopic simulators to their own unknown open-loop coarse-grained saddle points at a chosen value of the bifurcation parameter when no macroscopic/coarse-grained equations are available. The proposed procedure could serve at a low computational cost as an alternative to other branch-continuation techniques such as the pseudo-arc length continuation in order to trace bifurcation diagrams around regular turning points.

This is accomplished through the construction of a sequence of “control” actions, using the bifurcation parameter as an “actuator,” and designing its dynamics utilizing basic numerical bifurcation theory concepts. The procedure builds the actions through a chord-like method in order to drive the microscopic simulator around its own coarse-grained criticality, and finally steer it to the coarse-grained saddle point that is sought for a given configuration of the parameter space.

The procedure is illustrated using two microscopic simulations, namely (a) a kinetic Monte Carlo implementation of a simple surface reaction scheme for which the macroscopic equations for the expected values of the state variables were known so that we could
validate our results, and, (b) an agent-based model describing in a simplistic way the dynamics of many interacting “investors” under mimesis. Both models exhibit coarse regular turning points marking the onset of coarse-grained saddles.

Using the microscopic simulators as black box coarse-timesteppers, we were able to locate the coarse-grained saddles at specified values of the bifurcation parameters. We also constructed in an iterative way the expected open-loop coarse-grained bifurcation diagrams.

The methodology described here is not only applicable to multiscale/microscopic systems but also to very-large dynamical systems, modeled by ordinary and/or partial differential equations, as these arise in many fields such as material science, engineering, population dynamics, and biological problems. It may also possibly serve as a basis for the development of new adaptive control protocols that can be used to drive physical experiments directly to their own coarse-grained saddles.

The basic prerequisites of the approach are (a) the occurrence of a time-scale separation so that the detailed dynamics can be decomposed into fast and coarse grained slow ones, (and if this holds) (b) the a priori knowledge of the coarse-grained “slow” variables, and finally (c) a clear separation between time-scales between the unstable and stable coarse-grained modes (which is valid in a neighborhood of regular turning points).

The first assumption suggests that in principle, one can write down a system of macroscopic equations in the form of ordinary and/or partial differential equations, in terms of a few coarse-grained variables; however, the explicit derivation of such a model is most of the times, due to the inherent complexity, overwhelming difficult to derive in a closed form. The second assumption implies the knowledge of the “appropriate” observables. However, in several complex problems, these are not known beforehand. In this case, one should first resort to advanced techniques for data reduction such as Principal Component Analysis, or Diffusion Maps [85] that can suggest the right coarse-grained observables. The third assumption of the proposed methodology signifies a separation of times scales between the macroscopic modes. In particular, it implies the emergence of an effectively one-dimensional slow manifold around the criticality, which holds true in the proximity of a regular turning point. At this point, we should also note that the third assumption indicates that the saddle point that we want to reach is “close” to the turning point. If one wishes to reach saddle points far from the turning point (where the third assumption is not longer valid), he can do so by reaching two successive saddle points which are close to the turning point, and consequently apply a standard natural continuation technique.

Further research could also proceed toward the exploitation of the method in the case of disconnected branches as well as the connection of the method with techniques such as the Computational Singular Perturbation (CSP) [86] for the systematic numerical reconstruction of the slow manifolds. In that way, one would systematically converge to the slow manifold in the coarse-grained phase space, and thus relax the third assumption of the method.
Acknowledgements  This work was partially supported by the State Scholarships Foundation of Greece (IKY) and the National Technical University of Athens through the Basic Research Program “Constantine Caratheodory.”

References

1. Adalsteinsson, D., Sethian, J.: A level set approach to a unified model for etching, deposition, and lithography III: Re-deposition, reemission, surface diffusion, and complex simulations. J. Comput. Phys. 138, 193–223 (1997)
2. Alder, B.J., Wainwright, T.E.: Studies in molecular dynamics. I. General method. J. Chem. Phys. 31(2), 459 (1959)
3. Andersen, H.C.: Molecular dynamics simulations at constant pressure and/or temperature. J. Chem. Phys. 72, 2384–2393 (1980)
4. Frenkel, D., Smit, B.: Understanding Molecular Simulation: From Algorithms to Applications. Academic Press, San Diego (2002)
5. Gungor, M.R., Maroudas, D., Zhou, S.J.: Molecular dynamics study of the mechanism and kinetics of void growth in ductile metallic thin films. Appl. Phys. Lett. 77, 343–345 (2000)
6. Mendeleev, M.I., Han, S., Srolovitz, D.J., Ackland, G.J., Sun, D., Asta, M.: Development of new interatomic potentials appropriate for crystalline and liquid iron. Philos. Mag. B 83(35), 3977–3994 (2003)
7. Pantelides, D.M.S.T., Laks, D.B.: Defects in heterogeneous solids: from microphysics to macrophysics. Mater. Sci. Forum 143, 1–8 (1994)
8. Parinello, M., Rahman, A.: Crystal structure and pair potential: a molecular dynamics study. Phys. Rev. Lett. 45, 1196–1199 (1980)
9. Rapaport, D.C.: The Art of Molecular Dynamics Simulation. Cambridge University Press, Cambridge (1995)
10. Allen, M.P., Tildesley, D.J.: Computer Simulation of Liquids. Oxford University Press, London (1989)
11. Doi, M.: Molecular dynamics and rheological properties of concentrated solutions of rodlike polymers in isotropic and liquid crystalline phases. J. Polym. Sci., Part B, Polym. Phys. 19, 229–243 (1981)
12. Doi, M., Edwards, S.F.: The Theory of Polymer Dynamics. Clarendon Press, Oxford (1988)
13. Frisch, U., Hasslacher, B., Pomeau, Y.: Lattice-gas automata for the Navier-Stokes equation. Phys. Rev. Lett. 56, 1505–1508 (1986)
14. Larson, R.G.: The Structure and Rheology of Complex Fluids. Oxford University Press, New York (1999)
15. Padding, J., Boek, E., Briels, W.: Rheology of wormlike micellar fluids from Brownian and molecular dynamics simulations. J. Phys.: Condens. Matter 17, S3347 (2005)
16. Tao, Y., den Otter, W.K., Briels, W.J.: Kayaking and wagging of rods in shear flow. Phys. Rev. Lett. 95, 2378021-4 (2005)
17. Iori, G.: A microsimulation of traders activity in the stock market: the role of heterogeneity, agents? Interactions and trade frictions. J. Econ. Behav. Organ. 49, 269–285 (2002)
18. Liu, X., Gregor, S., Yang, J.: The effects of behavioral and structural assumptions in artificial stock market. Physica A 387, 2535 (2008)
19. Raberto, M., Cincotti, S., Focardi, S., Marchesi, M.: Agent-based simulation of a financial market. Physica A 299, 319–327 (2001)
20. Samanidou, E., Zschischang, E., Stauffer, D., Lux, T.: Agent-based models of financial markets. Rep. Prog. Phys. 70, 409–450 (2007)
21. Wang, S., Zhang, C.: Microscopic model of financial markets based on belief propagation. Physica A 354, 496–504 (2005)
22. Bressloff, P.C., Coombs, S.: Travelling waves in chains of pulse-coupled integrate-and-fire oscillators with distributed delays. Physica D 130, 232–254 (1999)
23. Casti, A.R.R., Omurtag, A., Sornborger, A., Kaplan, E., Knight, B., Sirovich, L., Victor, J.: A population study of integrate-and-fire-or-burst neurons. Neural Comput. 14, 957–986 (2002)
24. Coombs, S., Oshbaldestin, A.H.: Period-adding bifurcations and chaos in a periodically stimulated excitatory neural relaxation oscillator. Phys. Rev. E 62, 4057–4066 (2000)
25. Ermentrout, B.G., Chow, C.C.: Modeling neural oscillations. Physiol. Behav. 77, 629–633 (2002)
26. Kozma, R., Puljic, M., Balister, P., Bollobas, B., Freeman, W.J.: Phase transitions in the neuropercolation model of neural populations with mixed local and non-local interactions. Biol. Cybern. 92, 367–379 (2005)
27. Laing, C.R., Chow, C.: Stationary bumps in networks of spiking neurons. Neural Comput. 13, 1473–1494 (2001)
28. Laing, C.R., Chow, C.: A spiking neuron model for binocular rivalry. J. Comput. Neurosci. 12, 39–53 (2002)
29. Omurtag, A., Knight, B.W., Sirovich, L.: On the simulation of large populations of neurons. J. Comput. Neurosci. 8, 51–63 (2000)
30. Burke, D.S., Epstein, J.S., Cummings, D.A.T., Parker, J.I., Klime, K.C., Singa, R.M., Chakravarty, S.: Individual-based computational modeling of smallpox epidemic control strategies. Acad. Emerg. Med. 13, 1142–1149 (2006)
31. Eubank, S.H., Guclu, V.S.A., Kumar, M., Marathe, M.V., Srinivasan, A., Toroczkai, Z., Wang, N.: Modelling disease outbreaks in realistic urban social networks. Nature 429, 180–184 (2004)
32. Ferguson, N.M., Cummings, D.A.T., Cauchemez, S., Fraser, C., Riley, S., Meeyai, A., Iamsirithaworn, S., Burke, D.S.: Strategies for containing an emerging influenza pandemic in southeast Asia. Nature 437, 209–214 (2005)
33. Keeling, M.J., Eames, K.T.D.: Networks and epidemic models. J. R. Soc. Interface 2, 295–307 (2005)
34. Longini, I.M., Fine, P.E., Thacker, S.B.: Predicting the global spread of new infectious agents. Am. J. Epidemiol. 123, 383–391 (1986)
35. Bonabeau, E., Dorigo, M., Theraulaz, G.: Inspiration for optimization from social insect behaviour. Nature 406, 39–42 (2000)
36. DeAngelis, D.L., Rose, K., Huston, M.: Frontiers in Mathematical Ecology. Springer, Berlin (1994)
37. Grimm, V.: Ten years of individual-based modelling in ecology: what have we learned, and what could we learn in the future? Ecol. Model. 115, 129–148 (1999)
38. Levine, H., Rappel, W.J.: Self-organization in systems of self-propelled particles. Phys. Rev. E 63, 0171011-4 (2001)
39. Liu, Y., Passino, K.M.: Stable social foraging swarms in a noisy environment. IEEE Trans. Autom. Control 49, 30–44 (2004)
40. Balmer, M., Nagel, K., Raney, B.: Large scale multi-agent simulations for transportation applications. J. Intell. Transport. Syst. 8, 205–221 (2004)
41. Dijkstra, J., Jessurun, A., Timmermans, H.: Pedestrian and Evacuation Dynamics. Springer, Berlin (2001)
42. Helbing, D.: Traffic and related self-driven many-particle systems. Rev. Mod. Phys. 73, 1067–1141 (2001)
43. Low, D.J., Addison, P.S.: A nonlinear temporal headway model of traffic dynamics. Nonlinear Dyn. 16, 127–151 (1998)
44. Raney, B., Cetin, N., Volmy, A., Vrtic, M., Axhausen, K., Nagel, K.: An agent-based microsimulation model of swiss travel: first results. Netw. Spat. Econ. 3, 23–41 (2003)
45. Dhooge, A., Govaerts, W., Kuznetsov, Y.A.: MATCONT: A MATLAB package form numerical bifurcation analysis of ODEs. ACM Trans. Math. Softw. 29, 141–164 (2003)
46. Doedel, E.J., Govaerts, W., Kuznetsov, Y.A., Dhooge, A.: Numerical continuation of branch points of equilibria and periodic orbits. Int. J. Bifurc. Chaos 15, 841–860 (2005)
47. Doedel, E., Tuckerman, L.S. (eds.): Numerical methods for bifurcation problems and large-scale dynamical systems. IMA Volumes in Mathematics and its Applications, vol. 119. Springer, Berlin (2000)
48. Govaerts, J.: Numerical Methods for Bifurcations of Dynamical Equilibria. SIAM, Philadelphia (2000)
49. Parker, T.S., Chua, L.O.: Practical Numerical Algorithms for Chaotic Systems. Springer, New York (1989)
50. Seydel, R.: Practical Bifurcation and Stability Analysis: From Equilibrium to Chaos, 2nd edn. Springer, Berlin (1994)
51. Gear, C.W., Kevrekidis, I.G., Theodoropoulos, C.: Coarse integration/bifurcation analysis via microscopic simulators: micro-Galerkin methods. Comput. Chem. Eng. 26, 941–963 (2002)
52. Haataja, M., Srolovitz, D.J., Kevrekidis, I.G.: Apparent hysteresis in a driven system with self-organized drag. Phys. Rev. Lett. 92, 1606031–4 (2004)
53. Kevrekidis, I.G., Gear, C.W., Hyman, J.M., Kevrekidis, P.G., Runborg, O., Theodoropoulos, C.: Equation-free coarse-grained multiscale computation: enabling microscopic simulators to perform system-level tasks. Commun. Math. Sci. 1(4), 715–762 (2003)
54. Kevrekidis, I.G., Gear, C.W., Hummer, G.: Equation-free: the computer-assisted analysis of complex multiscale systems. AIChE J. 50(7), 1346–1354 (2004)
55. Makeev, A., Maroudas, D., Kevrekidis, I.G.: Coarse stability and bifurcation analysis using stochastic simulators: kinetic Monte Carlo examples. J. Chem. Phys. 116, 10083–10091 (2002)
56. Mooler, J., Runborg, O., Kevrekidis, P.G., Lust, K., Kevrekidis, I.G.: Equation-free, effective computation for discrete systems: a time stepper based approach. Int. J. Bifurc. Chaos Appl. Sci. Eng. 15(3), 975–996 (2005)
57. Moon, S.J., Ghanem, R., Kevrekidis, I.G.: Coarse graining the dynamics of coupled oscillators. Phys. Rev. Lett. 96(14), 144101–4 (2006)
58. Runborg, O., Theodoropoulos, C., Kevrekidis, I.G.: Effective bifurcation analysis: a stepper-based approach. Nonlinearity 15, 491–511 (2002)
59. Russo, L., Siettos, C.I., Kevrekidis, I.G.: Reduced computations for nematic-liquid crystals: a stepper approach for systems with continuous symmetries. J. Non-Newton. Fluid Mech. 146, 51–58 (2007)
60. Siettos, C.I., Graham, M., Kevrekidis, I.G.: Coarse Brownian dynamics for nematic liquid crystals: bifurcation diagrams via stochastic simulation. J. Chem. Phys. 118, 10149–10156 (2003)
61. Makeev, A.G., Maroudas, D., Panagiotopoulos, A., Kevrekidis, I.G.: Coarse bifurcation analysis of kinetic Monte Carlo simulations: a lattice-gas model with lateral interactions. J. Chem. Phys. 117, 8229–8240 (2002)
62. Siettos, C.I., Armaou, A., Makeev, A.G., Kevrekidis, I.G.: Microscopic/stochastic timesteps and coarse control: a kinetic Monte Carlo example. AIChE J. 49, 1922–1926 (2003)
63. Armaou, A., Siettos, C.I., Kevrekidis, I.G.: Time-steppers and coarse control of microscopic distributed processes. Int. J. Robust Nonlinear Control 14, 89–111 (2004)
64. Samaey, G., Vanroose, W., Roose, D., Kevrekidis, I.G.: Newton-Krylov solvers for the equation-free computation of coarse traveling waves. Comput. Methods Appl. Mech. Eng. 197(43–44), 3480–3491 (2008)
65. Kavousanakis, M., Russo, L., Siettos, C., Boudouvis, A.G., Georgiou, G.C.: A stepper approach for the systematic bifurcation and stability analysis of polymer extrusion dynamics. J. Non-Newton. Fluid Mech. 151, 59–68 (2008)
66. Siettos, C.I., Maroudas, D., Kevrekidis, I.G.: Coarse bifurcation diagrams via microscopic simulators: a state-feedback control-based approach. Int. J. Bifurc. Chaos Appl. 14, 207–220 (2004)
67. Siettos, C., Rico-Martinez, R., Kevrekidis, I.G.: A systems-based approach to multiscale computation: equation-free detection of coarse-grained bifurcations. Comput. Chem. Eng. 30, 1632–1642 (2006)
68. Christofides, P.D., Armaou, A.: Control and optimization of multiscale process systems. Comput. Chem. Eng. 30, 1670–1686 (2006)
69. Lou, Y.M., Christofides, P.D.: Feedback control of surface roughness in sputtering processes using the stochastic Kuramoto-Sivashinsky equation. Comput. Chem. Eng. 29, 741–759 (2005)
70. Ni, D., Christofides, P.: Dynamics and control of thin film surface microstructure in a complex deposition process. Chem. Eng. Sci. 60, 1603–1617 (2005)
71. Ni, D., Christofides, P.: Multivariable predictive control of thin film deposition using a stochastic PDE model. Ind. Eng. Chem. Res. 44, 2416–2427 (2005)
72. Gallivan, M.A., Murray, R.M.: Reduction and identification methods for Markovian control systems, with application to thin film deposition. Int. J. Robust Nonlinear Control 14, 113–132 (2004)
73. Braatz, R., Alkire, R., Seebauer, E., Rusli, E., Gunawan, R., Drews, X.L., T.O., H.E., Y.: Perspectives on the design and control of multiscale systems. J. Process Control 16, 193–204 (2006)
74. Rusli, E., Drews, T.O., Ma, D.L., Alkire, R.C., Braatz, R.D.: Robust nonlinear feedback-feedforward control of a coupled kinetic Monte Carlo—finite difference simulation. J. Process Control 16, 409–417 (2006)
75. Fenichel, N.: Geometric singular perturbation theory for ordinary differential equations. J. Differ. Equ. 31, 53–98 (1979)
Detection of coarse-grained unstable states of microscopic/stochastic systems: a timestepper-based

76. Kuznetsov, Y.A.: Elements of Applied Bifurcation Theory, 2nd edn. Springer, Berlin (1998)
77. Kelley, C.T.: Iterative Methods for Linear and Nonlinear Equations. SIAM, Philadelphia (1995)
78. Gillespie, D.T.: A general method for numerically simulating the stochastic time evolution of coupled chemical reactions. J. Comput. Phys. 22, 403–434 (1976)
79. Gillespie, D.T.: Exact stochastic simulation of coupled chemical reactions. J. Phys. Chem. 81, 2340–2361 (1977)
80. Ertl, G.: In: Anderson, J.R., Boudart, M. (eds.) Catalysis, Science and Technology, vol. 4. Springer, Berlin (1983). p. 209
81. Eiswirth, M., Ertl, G.: Kinetic oscillations in the catalytic CO oxidation on a Pt(110) surface. Surf. Sci. 177, 90–100 (1986)
82. Eiswirth, R.M., Krischer, K., Ertl, G.: Nonlinear dynamics in the CO-oxidation on Pt single crystal surfaces. Appl. Phys. A, Mater. Sci. Process. 51, 79–90 (1990)
83. Rosè, H., Hempel, H., Schimansky-Geier, L.: Stochastic dynamics of catalytic CO oxidation on Pt(100). Physica A 206, 42–440 (1994)
84. Omurtag, A., Sirovich, L.: Modeling a large population of traders: mimesis and stability. J. Econ. Behav. Organ. 61, 562–576 (2006)
85. Coifman, R.R., Lafon, S., Lee, A.B., Maggioni, M., Nadler, B., Warner, F., Zucker, S.: Geometric diffusions as a tool for harmonic analysis and structure definition of data. Part I: Diffusion maps. Proc. Natl. Acad. Sci. USA 102(21), 7426–7431 (2005)
86. Goussis, D., Valorani, M.: An efficient iterative algorithm for the approximation of the fast and slow dynamics of stiff systems. J. Comput. Phys. 214, 316–346 (2006)