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2012 EPL 99 48007

(http://iopscience.iop.org/0295-5075/99/4/48007)

A Letters Journal Exploring the Frontiers of Physics

August 2012

EPL, **99** (2012) 48007 www.epljournal.org
doi: 10.1209/0295-5075/99/48007

An equation-free approach to agent-based computation: Bifurcation analysis and control of stationary states

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received 19 March 2012; accepted in final form 17 July 2012
published online 29 August 2012

PACS 89.75.-k – Complex systems
PACS 89.65.-s – Social and economic systems
PACS 05.45.-a – Nonlinear dynamics and chaos

Abstract – We show how the equation-free approach can be exploited to enable agent-based simulators to perform system-level computations such as bifurcation, stability analysis and controller design. We illustrate these tasks through an event-driven agent-based model describing the dynamic behaviour of many interacting investors in the presence of mimesis. Using short bursts of appropriately initialized runs of the detailed, agent-based simulator, we construct the coarse-grained bifurcation diagram of the (expected) density of agents and investigate the stability of its multiple solution branches. When the mimetic coupling between agents becomes strong enough, the stable stationary state loses its stability at a coarse turning point bifurcation. We also demonstrate how the framework can be used to design a wash-out dynamic controller that stabilizes open-loop unstable stationary states even under model uncertainty.

Introduction. – Agent-based models are becoming the tools of choice for modelling many current complex real-world problems, ranging from ecology [1–3], epidemiology [4,5] and financial markets [6–8], to traffic and supply-chain networks [9], biological [10,11] and social systems [12–14]. Agents draw and process information from their external environment, communicate and interact with their neighbours and behave accordingly (move or stand, buy or sell, produce or consume, infect others or get vaccinated) via detailed, individual-based evolution rules. A persistent and fundamental feature of such models is that their emergent behaviour (macroscopic, population-level dynamical phenomena which arise from the interactions of individuals) cannot, most of the time, be trivially predicted from knowledge of the individual-based rules. In this paper we will use the term *coarse-grained* or *coarse* to refer to this type of emergent behaviour and its features (*e.g.*, its bifurcation diagrams).

Efficient modelling/computational tools for the system-level analysis of agent-based model behaviour requires coarse-grained models in closed form. Traditionally, the aggregate dynamics of the stochastic agent-based simulations are modelled using analytical techniques (such as mean-field and pair-wise approximations, Master or Fokker-Planck equations) from which macroscopic evolution equations can be obtained for a few leading moments of the underlying agent distribution. These approaches involve the derivation of relations between coarse-grained variables (typically moments of the underlying detailed distribution). However, no general systematic methodology for deriving such closures exists; they are often based on assumptions (such as infinite population and homogeneity of agents, homogeneous contact network characteristics) that may introduce biases in the analysis (*e.g.*, see the discussion in [15]). Hence, finding good closures relating higher-order moments to lower-order ones constitutes a major stumbling block in contemporary agent-based modelling and analysis.

Here, we show how the *equation-free approach* [16,17] can be exploited to analyse in a systematic way the coarse-grained, emergent dynamics by linking individual-based simulation with established continuum numerical analysis and control methods. The main idea of this "numerical analysis assisted" framework is to sidestep the explicit derivation of population-level equations through the use of appropriately initialized short bursts of the agent-based

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simulator; these help estimate on demand (as opposed to obtaining from explicit formulas) the quantities required in continuum numerics (coarse residuals, the action of coarse Jacobians, control matrices etc.). In particular we demonstrate how the equation-free concept reviewed in [16,17] can be applied to perform coarse-grained bifurcation analysis and coarse controller design for washing out model uncertainty.

Our illustrative example is a simple but informative event-driven, financially motivated model developed by Omurtag and Sirovich [6]. They simulated the behaviour of a large population of investors each of which buys or sells on the basis of information from the external environment as well as from the actions of other agents.

Treating the event-driven agent-based simulator as a black box we will construct the coarse bifurcation diagram of the agent distribution with respect to a (bifurcation) parameter quantifying the strength of interactions between agents. We will show that the explosive instability (a caricature of a "bubble") observed in the dynamics is, in effect, a coarse saddle-node bifurcation. This is associated with an unstable branch of coarse stationary solutions, which simply cannot be reached through long-time direct temporal simulations. We will also design, within the equation-free framework, a linear wash-out dynamic controller [18,19] that stabilizes the open-loop unstable system stationary states even under model uncertainty.

The agent-based model: a financial caricature model. – Our illustrative model (see [6]) consists of a set of identical agents, each with an internal state indicating its propensity to buy or sell. The state is a real numerical value in $(-1,\ 1)$. Each agent "listens to" the exogenous "good" as well as "bad" news sources; information from these sources "arrives" randomly to each agent with Poisson rates ν_{ex}^{+} and ν_{ex}^{-}, respectively. When a quantum of good (bad) information is perceived by an agent, it reacts by increasing its state by ϵ^+ (decreasing it by ϵ^-). The state of each agent thus changes, in an event-driven manner, via a series of positive or negative jumps at times $t^{(k)}$, $k=1,2,3,\ldots$. Between these times —that is, in the absence of any new information— each agent's state drifts towards zero: it decays exponentially with rate constant γ. If an agent's state ever exceeds $+1$ or falls below -1, the agent immediately "buys" or "sells" and its state is reset to zero.

Importantly, agents are also influenced by the perceived overall buying and selling rates. We denote these variable rates (which depend on the evolving system state) by R^+ and R^-: they are defined as the fraction of agents buying or selling per unit time. Their effect is to increase the apparent arrival rates of (good as well as of bad) news. A system parameter, g, quantifies these buying/selling rate effects on the apparent information arrival rates. These rates are now

$$\nu^{\pm}=\nu_{ex}^{\pm}+gR^{\pm}. \tag{1}$$

Since the buys and sells are discrete events, we define the buying and selling rates as averages over a small, finite interval, say δT (that we call the *reporting horizon*); a physical interpretation is that gross activity is not broadcast instantaneously, but is instead reported at regular intervals. Thus, the state X_i of each individual in the model evolves within $(-1,\ 1)$. After one agent buys (sells) the probability of all other agents buying (selling) increases in the next reporting interval. The above formulation bears strong analogies to integrate-and-fire models of neurons [6,20].

By retaining terms through second order in a power series in terms of the jump magnitudes (ϵ^+ and ϵ^-) Omurtag and Sirovich provide in [6] a Fokker-Planck–type approximation for the evolution of the probability density of their agents:

$$\frac{\partial\rho}{\partial t}=\frac{\partial(\mu\rho)}{\partial X}+\frac{1}{2}\sigma^2\frac{\partial^2\rho}{\partial X^2}+(R^++R^-)\delta(X), \tag{2}$$

where $\sigma^2(t)=\nu^+(\epsilon^+)^2+\nu^-(\epsilon^-)^2$ and $\mu(X,t)=\gamma X-(\nu^+\epsilon^++\nu^-\epsilon^-)$.

The buy/sell rates are now $R^{\pm}=\mp\frac{1}{2}\sigma^2\partial\rho/\partial X\,|_{X=\pm1}$.

The boundary conditions read: $\rho(X=\pm1,t)=0$ and the total probability is conserved, *i.e.*, $\int_{-1}^{1}\rho(X,t)\,\mathrm{d}X=1$.

A simple way to compute steady states of eq. (2) is to solve the boundary value problem obtained by setting the time derivative equal to zero. This gives a reasonable approximation of the stationary states of the actual agent-based simulation. It should be noted that the solution of eq. (2) is smooth except for a discontinuous derivative at the origin (see [6]).

Using the agent-based model with a relatively large number of agents (50000) and nonzero ϵ^+ and ϵ^- we attempt to find the stationary density of the simulated agent states. The general approach we use for such problems is to represent the data at two distinct levels: the "microscopic" individual-based level (the state of each agent) and the "macroscopic", coarse-grained level (a discretisation of the agent state density). We create mappings between these two representations: a) the *restriction operation* that observes the microscopic state at the macroscopic level (*e.g.*, obtains discretised agent state densities from agent states) and its reverse, b) the (one-to-many) *lifting operation* which creates agent state realizations with prescribed density profiles. When the microscopic process is a stochastic one (as in this example) we lift to an ensemble of such consistent realizations.

Equation-free multiscale computations: the coarse timestepper. – We start with a brief description of coarse timesteppers and the framework for coarse-grained bifurcation calculations and coarse controller design (see fig. 1). Coarse timesteppers [16,17] provide a bridge between microscopic/stochastic modelling, on the one hand, and traditional, continuum numerical algorithms on the other, and consist of the following essential steps:

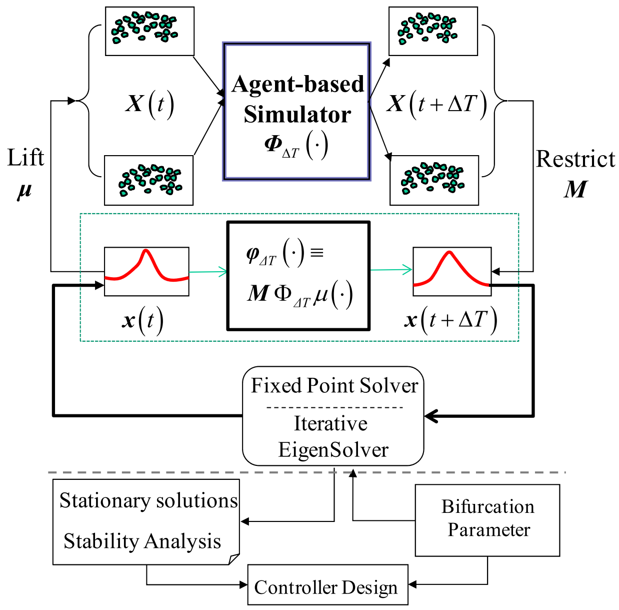

Fig. 1: (Colour on-line) Schematic of the coarse timestepper.

a) *Start from a macroscopic initial condition, corresponding to the appropriate statistic* $\boldsymbol{x}(t)$ *(typically low-order moments) of the evolving individual agent distributions at time* t.

b) *Map this macroscopic description,* $\boldsymbol{x}(t)$*, through a lifting operator,* $\boldsymbol{\mu}$*, to an ensemble of consistent microscopic realizations (agent distributions)*:

$$\boldsymbol{X}(t) = \boldsymbol{\mu x}(t). \tag{3}$$

c) *Evolve these realizations using the agent-based simulator for an (appropriately chosen) short macroscopic time* ΔT*, to obtain the value(s)*:

$$\boldsymbol{X}(t+\Delta T) = \boldsymbol{\Phi}_{\Delta T}(\boldsymbol{X}(t)) \equiv \boldsymbol{\Phi}_{\Delta T}(\boldsymbol{\mu x}(t)); \tag{4}$$

the choice of ΔT *is driven by estimates of the separation of time scales between the individual agent dynamics and the coarse-grained dynamics* [16].

d) *Map the (ensemble of) individual distributions back to the macroscopic description through the restriction* $\boldsymbol{M}$

$$\boldsymbol{x}(t+\Delta T) = \boldsymbol{M X}(t+\Delta T); \tag{5}$$

lifting from macroscopic to microscopic and then restricting back should have no effect on the coarse variables, that is, $\boldsymbol{M\mu} = \boldsymbol{I}$.

This procedure can be thought of as a "black box"

$$\boldsymbol{x}(t+\Delta T) = \boldsymbol{\phi}_{\Delta T}[\boldsymbol{x}(t)], \tag{6}$$

where $\boldsymbol{\phi}_{\Delta T}(.) \equiv \boldsymbol{M\Phi}_{\Delta T}(\boldsymbol{\mu}(.))$. We now "wrap" around the coarse timestepper matrix-free computational superstructures like a) Newton-GMRES [21] to find the fixed points of eq. (6); or b) Arnoldi iterative algorithms [22] for estimating the dominant eigenvalues of the coarse linearization, quantifying the stability of the steady states of the unavailable macroscopic evolution equations.

This computational framework serves as an *on demand* identification methodology for right-hand sides, action of coarse Jacobians, coarse derivatives with respect to parameters etc.; in short, exactly the quantities that a traditional numerical bifurcation code would evaluate through explicit macroscopic model formulas. The analogy carries over to control and even optimization computations: coarse timesteppers can also become a bridge between agent-based models and traditional continuum controller design techniques (pole placement, optimal and/or nonlinear control methodologies) [23,24].

The key assumption underlying the entire framework is that a coarse description exists *in principle*: higher-order moments of the evolving distributions become rapidly (over a few characteristic interaction times in an agent-based simulation) slaved to the lower-order ones, evolving quickly towards a slow manifold parameterised by these slow moments. This is the singularly perturbed system paradigm, where the set of coupled nonlinear ODEs for the agent distribution moments quickly approaches a low-dimensional slow manifold (see [16] for details).

Constructing the coarse-grained bifurcation diagram: simulation results. – In our illustrative simulations we used 50000 agents and the following values for the model parameters: $\epsilon^+ = 0.075$, $\epsilon^- = -0.072$, $\nu^+_{ex} = \nu^-_{ex} = 20$ and $\gamma = 1$. The reporting horizon was set to $\delta T = 0.25$ time units and the coarse time step ΔT was set equal to $4\delta T$. Because there is a greater propensity to buy rather than sell for larger values of g, this propensity becomes increasingly amplified, and it soon becomes clear that for large enough g the system will destabilize. We want to find the critical value and the nature of the instability.

At the macroscopic level we approximate the distribution of the agent states through its cumulative distribution function (CDF), discretised in a sufficient number (here, 37) of piecewise linear segments; the selected 37 percentile points x_i are denser at the distribution tails, where accuracy is important for the calculation of the buy and sell rates. Our coarse-grained variables are the 37 $x_i(t)$'s plus $R^+(t)$ and $R^-(t)$, *i.e.*, a total of 39 variables. The emergent dynamics of the system at the chosen parameter values are nontrivial: starting the simulations with all agents at the neutral position ($\boldsymbol{X}(t=0) = \boldsymbol{0}$), and for low values of the influence factor g, the system typically approaches stable stationary states. For larger values of g the buying rate appears to eventually blow up in finite time (see fig. 2).

These observations suggest that the system has a critical point (somewhere between $g = 45$ and $g = 47$) below which the behaviour appears stable and above which some sort of explosive instability sets in. To explore this apparent nonlinear dynamic instability we constructed

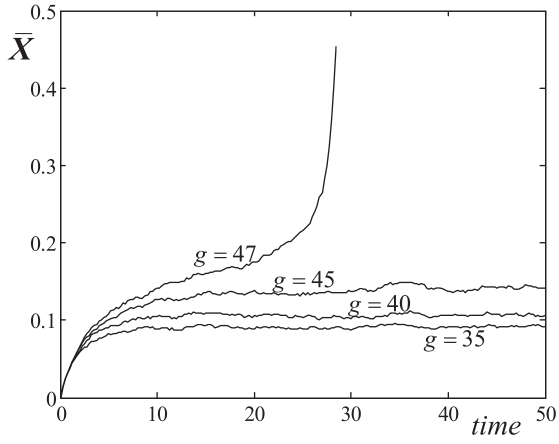

Fig. 2: Temporal simulations illustrating the evolution of the mean value of the agent state as the bifurcation parameter g varies. The results are indicative of the existence of a critical parameter value, marking the onset of a qualitative transition in the emergent dynamics.

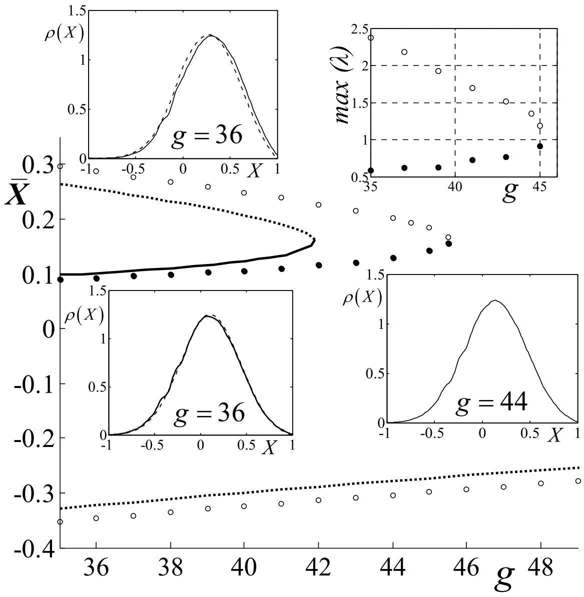

Fig. 3: Coarse bifurcation diagram computed through Newton-GMRES for the fixed points of the coarse timestepper with 50000 agents, 4000 copies, $\Delta T = 4\delta T$. Filled circles correspond to coarse-grained stable (node) states, while open circles correspond to coarse-grained unstable (saddle) states. The solution branches obtained from the PDE approximation given by eq. (2) are also shown for comparison purposes. Now solid (dotted) lines correspond to stable (unstable) states. The lower branch is unstable everywhere. The upper right inset depicts the growth of the largest coarse eigenvalue with respect to the bifurcation parameter. Representative coarse-grained stationary distributions at various values g, obtained through coarse equation-free computations (solid lines) as well as from the PDE solution (dotted lines), are shown as insets.

the coarse bifurcation diagram of the agent-based model using the equation-free methodology. Figure 3 shows the resulting detailed one-parameter coarse-grained bifurcation diagram in terms of the first-order moment (the mean value) of the stationary agent state distribution as a function of g. The stationary states in this diagram have been obtained as fixed points of the coarse agent-based timestepper averaged over 4000 realizations through the Newton-GMRES solution of

$$\boldsymbol{x} - \boldsymbol{\phi}_{\Delta T}(\boldsymbol{x}) = \boldsymbol{0}, \tag{7}$$

where as described above $\boldsymbol{x} = [x_1, x_2, \ldots, x_{37}, R^+, R^-]$. Their shape and stability are consistent with long-term agent-based simulations. Continuation around the turning point is accomplished by augmenting the fixed point equations with a pseudo-arclength condition:

$$\begin{aligned} N(\boldsymbol{x}, g) \; = \; & \frac{(\boldsymbol{x}_1 - \boldsymbol{x}_0)^T}{\delta s} \cdot (\boldsymbol{x} - \boldsymbol{x}_1) \\ & + \frac{(g_1 - g_0)}{\delta s}(g - g_1) - \delta s = 0, \end{aligned} \tag{8}$$

where $(\boldsymbol{x}_1, g_1)$ and $(\boldsymbol{x}_0, g_0)$ are two previously computed solutions and δs the pseudo-arclength increment. Filled circles correspond to stable coarse steady states while open circles depict unstable (saddle) states. The critical coarse eigenvalues are computed by wrapping the matrix-free Arnoldi iterative eigensolver around the coarse timestepper. The dependence of the leading one on the bifurcation parameter is included in the upper right inset of fig. 3; the turning point occurs when this eigenvalue crosses the unit circle at 1.

The coarse-grained turning point (around $g = 45.6$) marks the barrier between coarse stable (lower branch) and unstable (upper branch) open-loop equilibria; a second, isolated branch of unstable solutions is also followed in the diagram.

The bifurcation diagram as obtained from the partial differential equations (PDE) approximation given by eq. (2) is also shown for comparison purposes. Solid lines correspond to stable states and dotted ones correspond to unstable states. Clearly the "true" coarse-grained bifurcation diagram, computed through the coarse timestepper is qualitatively comparable *but quantitatively different* from the one computed by the PDE approximation: the critical point was found around $g = 45.6$, while the PDE approximation gives a critical point around $g = 42$. This suggests that the assumptions used to extract explicit macroscopic equations may impose systematic bias in the predictions of true emergent agent dynamics.

A control problem: equation-free stabilization of an unstable coarse-grained equilibrium. – Starting at an unstable coarse equilibrium, and depending on infinitesimal perturbations, open-loop dynamics can drive the system either to a coarse stable equilibrium or to solutions apparently blowing up in finite time (fig. 4).

We now design a controller that stabilizes such coarse unstable stationary states in the presence of uncertainty (ignorance of the appropriate stationary state, due to the

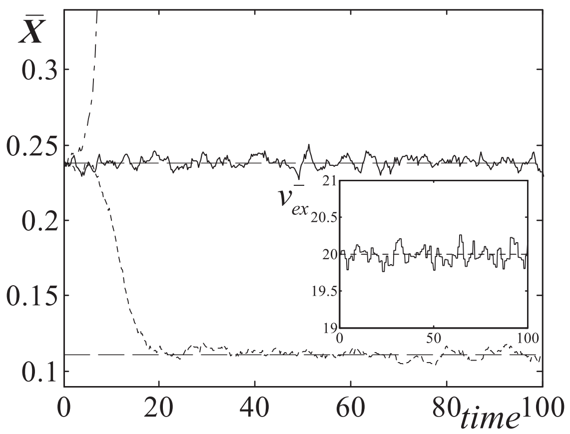

Fig. 4: Use of a dynamic controller to stabilize a coarse unstable equilibrium (here at $g=41$). Starting from the coarse-grained saddle, *open-loop* transients are either attracted to the coarse-grained stable equilibrium or blow up. The dynamic controller stabilizes the system to the "correct" coarse open-loop unstable equilibrium. The response of the control variable is also shown in the inset. The dashed lines correspond to the nominal coarse stationary states.

lack of explicit macroscopic equations). We denote these (unknown) macroscopic equations in the general discrete-time autonomous nonlinear system form,

$$\boldsymbol{x}_{k+1}=\boldsymbol{f}(\boldsymbol{x}_k,\ u_k),\quad \boldsymbol{f}\colon R^n\times R\to R^n, \tag{9}$$

where $\boldsymbol{x}\in R^n$ denotes the state vector of the coarse-grained variables, $u\in R$ is the control variable (here, this variable is ν_{ex}^-) and $\boldsymbol{f}(.)$ is the not-explicitly-available macroscopic evolution operator. To cope with this uncertainty we use *dynamic state feedback*, in contrast to static state feedback which would most likely be applied if the coarse-grained operating equilibrium was precisely known. Denote with $(\boldsymbol{x}_0,u_0)$ the "correct" coarse equilibrium of (9) and with $(\boldsymbol{x}^*,u_0)$ our best approximation of it. Our dynamic coarse-grained control law (a *"wash-out filter"*) reads

$$u_k=u_0+\boldsymbol{K}^T(\boldsymbol{x}_k-\boldsymbol{x}^*)+Dw_k, \tag{10}$$

where $w_k\in R$ satisfies

$$w_{k+1}=w_k+\boldsymbol{K}^T(\boldsymbol{x}_k-\boldsymbol{x}^*)+Dw_k. \tag{11}$$

The gains $\boldsymbol{K}$, D are selected so that local stabilization of eq. (9) is attained. This is typically shown by linearizing (9) around its fixed point, obtaining

$$\begin{aligned}\boldsymbol{x}_{k+1} &= \boldsymbol{x}^*+\left.\frac{\partial\boldsymbol{f}(\boldsymbol{x}_k,u_k)}{\partial\boldsymbol{x}_k}\right|_{(x^*,u_0)}(\boldsymbol{x}_k-\boldsymbol{x}^*)\\ &\quad+\left.\frac{\partial\boldsymbol{f}(\boldsymbol{x}_k,u_k)}{\partial u_k}\right|_{(x^*,u_0)}(u_k-u_0),\end{aligned} \tag{12}$$

compactly written as

$$\hat{\boldsymbol{x}}_{k+1}=\boldsymbol{A}\hat{\boldsymbol{x}}_k+\boldsymbol{B}\hat{u}_k \tag{13}$$

with $\hat{\boldsymbol{x}}_k=\boldsymbol{x}_k-\boldsymbol{x}^*, \hat{u}_k=u_k-u_0$, $\boldsymbol{A}=\frac{\partial\boldsymbol{f}(\boldsymbol{x}_k,u_k)}{\partial\boldsymbol{x}_k}|_{(x^*,u_0)}$, $\boldsymbol{B}=\frac{\partial\boldsymbol{f}(\boldsymbol{x}_k,u_k)}{\partial u_k}|_{(x^*,u_0)}$. After $\boldsymbol{A},\boldsymbol{B}$ are estimated through coarse timestepping computations, the augmented —with the dynamic controller— linearized system is given by

$$\begin{pmatrix}\hat{\boldsymbol{x}}_{k+1}\\ w_{k+1}\end{pmatrix}=\begin{pmatrix}\boldsymbol{A} & \boldsymbol{0}\\ \boldsymbol{0} & 1\end{pmatrix}\begin{pmatrix}\hat{\boldsymbol{x}}_k\\ w_k\end{pmatrix}+\begin{pmatrix}\boldsymbol{B}\\ 1\end{pmatrix}\hat{u}_k \tag{14}$$

and closing the loop using eqs. (10), (11) we obtain

$$\begin{pmatrix}\hat{\boldsymbol{x}}_{k+1}\\ w_{k+1}\end{pmatrix}=\begin{pmatrix}\boldsymbol{A}+\boldsymbol{B}\boldsymbol{K}^T & \boldsymbol{B}D\\ \boldsymbol{K}^T & 1+D\end{pmatrix}\begin{pmatrix}\hat{\boldsymbol{x}}_k\\ w_k\end{pmatrix}. \tag{15}$$

The dynamic response of eq. (15) can be shaped by properly prescribing the controller gains $\boldsymbol{K}$, D, through, *e.g.*, pole placement or discrete linear quadratic regulator (LQR) techniques [25]. Then, the control law (10), (11) "washes-out" the model uncertainty and drives the original system (9) to the "correct" steady state $(\boldsymbol{x}_0,u_0)$ since, $\boldsymbol{x}_{k+1}=\boldsymbol{x}_k$ and $w_{k+1}=w_k$ as $t\to\infty$ and, thus $u=u_0$ and $\boldsymbol{x}=\boldsymbol{x}_0$. Here we used a discrete LQR technique to select the optimal gain matrices $\boldsymbol{K}$, D such that the state feedback control law (10), (11) minimizes the cost function

$$J=\sum_{k=0}^{\infty}(\boldsymbol{x}_k^T\boldsymbol{Q}\boldsymbol{x}_k+u_kRu_k) \tag{16}$$

subject to the state dynamics; we chose $\boldsymbol{Q}=0.1\boldsymbol{I}_{39}$, $R=1$. The closed-loop response is depicted in fig. 4. Clearly, the controller succeeds in (locally) stabilising the dynamics around the initially unknown, unstable coarse-grained state.

Conclusions. – We have demonstrated, in a financial model caricature, that the equation-free computational methodology can be used to analyze important features of the macroscopic, emergent behaviour of agent-based models. While the example is admittedly simple, it does illustrate the scope of system-level tasks that one can attempt by acting directly on the agent-based simulation: stability, bifurcation analysis, as well as control tasks have been demonstrated here; coarse projective integration as well as coarse-grained optimization can also be attempted [26]. Note that nonlinear controller design approaches can also be formulated within our framework [27]. The tasks illustrated in this paper exploited the smoothness in time, in phase space, and in parameter space of the unavailable macroscopic equations in order to estimate time derivatives, functional derivatives, and derivatives with respect to the parameters for the correct macroscopic observables. It is also possible to use smoothness in space of the evolving distributions, so that the macroscopic simulation need only be performed in small, appropriately connected spatial domains ("teeth", separated by "gaps", giving rise to the so-called gap-tooth scheme and patch dynamics [16,28,29]. It is also important to note that here we started with a good idea of what the right macroscopic observables are (the single agent state distribution) —the variables in the unavailable macroscopic evolution equation. When these are not known *a priori*, techniques for data reduction (such as principal component analysis (PCA), kernel or nonlinear PCA) [30,31] can be used to suggest the right observables from simulations of the system itself, and can be naturally connected with our equation-free methodology [32].

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This work was partially supported by AFOSR (Award No. FA9550-09-0018) and the US Department of Energy (DE-SC000207). CIS gratefully acknowledges the support of a Fulbright Fellowship.

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