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Abstract phase space networks describing reactive dynamics

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HIGHLIGHTS

- A novel abstract network approach to describe spatiotemporal reactive processes.
- Proposed approach is applicable to any reactive system, with and without diffusion.
- Current approach is extendable in higher dimensions and different coordination numbers.
- Knowing system's phase space trajectories suffices for abstract network construction.
- Lattice Limit Cycle model: corresponding phase space abstract network is scale free.

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ABSTRACT

An abstract network approach is proposed for the description of the dynamics in reactive processes. The phase space of the variables (concentrations in reactive systems) is partitioned into a finite number of segments, which constitute the nodes of the abstract network. Transitions between the nodes are dictated by the dynamics of the reactive process and provide the links between the nodes. These are weighted networks, since each link weight reflects the transition rate between the corresponding states–nodes. With this construction the network properties mirror the dynamics of the underlying process and one can investigate the system properties by studying the corresponding abstract network. As a working example the Lattice Limit Cycle (LLC) model is used. Its corresponding abstract network is constructed and the transition matrix elements are computed via Kinetic (Dynamic) Monte Carlo simulations. For this model it is shown that the degree distribution follows a power law with exponent -1, while the average clustering coefficient $c(N)$ scales with the network size (number of nodes) N as $c(N) \sim N^{-\nu}$, $\nu \simeq 1.46$. The computed exponents classify the LLC abstract reactive network into the scale-free networks. This conclusion corroborates earlier investigations demonstrating the formation of fractal spatial patterns in LLC reactive dynamics due to stochasticity and to clustering of homologous species. The present construction of abstract networks (based on the partition of the phase space) is generic and can be implemented with appropriate adjustments in many dynamical systems and in time series analysis.

1. Introduction

A large variety of natural, technological and social systems which require cooperation between many individual units operate in the form of networks. Depending on the type of exchange between the network nodes, two important network

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categories are distinguishable: the spatial networks and the social networks [1,2]. Spatial networks are characterised by matter exchange between their nodes. Typical spatial networks are the large infrastructure networks, such as the transportation network, the road-map network, the airline and railway networks, electricity distribution network, and water-pipe networks [3,4]. An important class of spatial networks is the biological networks, which include the neuron networks, the blood vessels networks, the bronchial tree, the plant root network, etc. In the second major category, the social networks information is shared and exchanged between nodes. This category includes the Internet, Facebook, LinkedIn, Twitter, the authors network, the actors network, the classmates networks, etc. [3,5]. Both above categories have received considerable attention and are presented extensively in several review papers and books in the past 15 years (see Refs. [1,2,6,7]).

A third category, which has received less attention is the "state-space" networks or the "phase–space" networks. This category accounts for systems transiting between various states and are often associated with time series [8–10]. For such systems we can define the corresponding "abstract networks" whose nodes are the different states and whose links are the transitions rates from one state to another. As such, the abstract networks are classified in the class of weighted networks, since the links between the various states/nodes are weighted by the transition probabilities. The current study focuses on the properties of the abstract state network representing a reactive system, when its continuous phase space is segmented into a discrete number of nodes (network of states).

In previous studies abstract networks which result from the dynamics of symbol sequences with specific applications in DNA sequences, in motif recognition and in chaotic maps have been considered [11,12]. These networks are based on discrete state spaces which consist of finite sequences of symbols. The nodes are identified with finite symbol combinations or with specific motifs, while the links are identified either with proximity [11] or with coexistence [12] of the various motifs. Abstract networks in the form of graphs have also been studied in connection to biological and chemical processes as early as 1970s [13]. The graph theory was used in Ref. [13] for the solution of the master equation, describing the transitions of two models (chemical Schlögl model and biological membrane pore model) between their discrete state spaces. Both models involve a single variable and they are described at the Mean Field (MF) level.

Unlike in the above cases, in the current study the state space (phase space) is continuous. In reactive dynamics where a number of species n are involved, with species concentrations $x_i,\ i = 1, \ldots, n$, the phase space is n-dimensional. Normally, the concentration variables are normalised (partial concentrations), and thus x_i's are continuous variables which can take values in the range $0 \leq x_i \leq 1$. Since network theory is based on a finite number of nodes, the n-dimensional phase space needs to be appropriately partitioned, as will be discussed in Section 2.

As working reactive model the Lattice Limit Cycle (LLC) is used. The LLC model belongs to the class of predator–prey systems with the additional features that (a) it possesses a stable limit cycle with dissipative global oscillations of the species concentrations at the MF level and (b) it is lattice compatible, i.e. it can be directly implemented on a lattice conserving the number of lattice sites, without the need to modify its dynamics [14–17]. The phase space of LLC is 3-dimensional initially, but it is reduced to 2-dimensional due to the lattice compatibility condition. It is implemented here via Kinetic Monte Carlo (KMC) simulations where stochastic effects and local interactions are taken into account. The lattice KMC realisations of this model give rise to fractal spatial patterns which spontaneously form due to the cooperation of the nonlinearity of the interactions and the spatial restrictions.

The reason for using the LLC model as an example for the construction of the phase space abstract network is the complex fractal patterns which are formed during the system's evolution and which could give rise to nontrivial transition rates among the nodes of the corresponding abstract network. As it will be shown in the next sections the elements of the transition matrix have a long range distribution and the abstract network belongs to the class of scale free networks [1,6,18].

In the next section we propose and describe the abstract network representation of the reactive processes. In Section 3 the general features of the LLC reactive system are recapitulated, both at the MF level and using KMC simulations to account for spatial and stochastic effects. In Section 4 we calculate the abstract network transition matrix, the degree distribution and the average clustering coefficient which demonstrate the network's scale free character. Finally, we recapitulate the main results in the concluding section and we discuss open problems.

2. Abstract networks of reactive dynamical systems

The term *abstract networks in reaction–diffusion systems* proposed and developed here should *not* be confused with the classical field of "Chemical Reaction Networks" which has a long research history, mostly in Theoretical Chemistry [19,20]. In the classical literature scientists refer to a "network of chemical reactions" or to a "Chemical Reaction Network" (CRN) as a finite set of reactions among a finite set of chemical species. In CRNs often the products of one reaction serve as reactants in others. CRNs find multiple applications in Biochemistry and Analytical Chemistry and even in Catalysis [21–23]. The classical CRNs, in their spatial representations, can also serve under certain conditions as a reaction (or reaction–diffusion) system for the construction of the corresponding abstract network as will be described in the sequel.

In the present study we consider an abstract network of nodes, each node being an appropriately chosen segment of the state space of a reaction–diffusion system. Thus the dynamics of the system is mirrored on the transitions of the network from one part of the state space to another. To be more precise, consider a number n of reactants $X_i,\ i = 1, \ldots, n$ involved in a number of reactions. The reactive scheme for the time being need not be explicitly written and it can involve any number of reactions; even one reaction is enough for the definition of the abstract network. During the reactive process the various species X_i are represented by respective partial concentrations. These partial concentrations change with time and they are