Spreading dynamics in heterogenous media

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I. INTRODUCTION

Reaction-diffusion (RD) dynamics are ubiquitous processes that show up as soon as diffusing elements, when propagating in a general media, get close and react, modifying their state. Since reaction-diffusion dynamics are present in very different systems, the appropriate metodologies to achieve a good description of the systems could be very different. In some cases could be opportune to represent single individual moving and interacting in a media over which the dynamics occurs (agent based description), in other cases the process can be described via continuous fields by mesoscopic and coarse-grained approaches, like master equation or partial differential equation (PDE) description. The first presentation of RD problems with PDE approach dates back to 1937 with the studies of Fischer, Kolmogorov, Petrosvkii and Piskunov [1] regarding the autocatalytic reaction ($A + B \to 2A$). The problem is described by a PDE

$$\partial_t \theta(x,t) = D\Delta\theta(x,t) + \alpha f(\theta(x,t))\,, \tag{1}$$

where D is the molecular diffusivity, α is the reaction rate and $f(\theta)$ is a convex function ($f''(\theta) < 0$ and $f'(0) = 1$) with $f(0) = f(1) = 0$, which describes the reaction process. With this choice $\theta = 0, 1$ are the unstable and stable steady states of the reactive dynamic, respectively. The scalar field θ represents the fractional concentration of the reaction products: $\theta = 0$ indicates the fresh (unstable) material, $\theta = 1$ the inert (stable) one, and $0 < \theta < 1$ means that fresh materials coexist with products. In such a system, provided that the initial concentration is zero apart from a small portion of the system where $\theta \neq 0$, at long times one observes a front connecting unstable and stable states propagating through the space, i.e., $\theta(x,t) = h(x - v_f t)$, and $h(z) \sim e^{-z/\xi}$. The speed of the propagating front at long times reaches an asymptotic value, $v_0 = 2\sqrt{D\alpha}$, and the thickness of the active zone is $\xi = 8\sqrt{D/\alpha}$.

Later, reaction-transport dynamics attracted a considerable interest for their relevance in a large number of chemical, biological and physical systems [2–4]: the transport operator $D\Delta\theta$ has been extended in order to consider both moving media [5] (reaction-diffusion-advection problem) and anomalous diffusion, and the reaction term $f(\theta)$ has been generalized in order to consider various kinds of interaction between different species (logistic model, model with Allee effect). Within this framework it is possible to study many different problems like spreading and invasion in heterogeneous media.
The main theme of the work in my first PhD year is related to the study of reaction diffusion processes on complex networks.

The study of complex networks is a recent discipline that gathers together methods from both graph theory and statistical mechanics. As a result it provides a playground for the investigation

of systems coming from different disciplines ranging from physics to social science and from biology to computer science [6–9].

Networks are mathematically described using graphs with different features. A graph is a set of nodes ($i \in V$, $i = 1, ..., N$) , or vertex, connected by links or edges, $(i, j) \in E$, fully defined by its adjacency matrix [10], A_{ij}, that is equal to 1, or 0, if the link (i, j) is in E (for graph with non-weighted links) , or not.

The connectivity of a node, k_i, also known as degree of node i, is equal to the number of connections starting from the node $k_i = \sum_j A_{ij}$. There are different types of graphs, from simple ones, like lattices or sites connected only with their nearest neighbor, to widely studied random graphs. The first model of this type is the Erdös-Renyi [11] model where a connection between two nodes exist with probability p. Random graphs provide flexible models to study complex structure of interaction and transmission of information.

Many researchers have studied the dynamics of systems living in a network is of great interest in many contexts [8, 9], highlighting the importance of dynamical processes on complex networks (e.g., we can mention the works on the epidemic spreading [12], or those on the spreading patterns of mobile phone viruses [13], or the signal propagation in the protein [14]). Moreover in chemistry, biology and social science one has to deal with active species in non-trivial substrates [2]. In particular, in biological systems a completely new focus have been posed on the complex networks due to the ubiquitous appearance of network structure in living systems (gene networks, protein interaction networks, predator-prey interaction) [15]. An accurate description of networks dynamics concern numerical simulations in which the graph structure of the network is entirely considered. The first studies of my project of thesis deal with RD field dynamic on graphs [16], trying to relate the topological properties of graphs with dynamical behavior of the system.

RD on graphs

In order to extend Eq. (1) to non homogeneous media (i.e. networks), so to study spreading problem with a PDE approach on heterogenous media, as first it is necessary to generalize the diffusion term, $D\Delta\theta$. For example, the discrete diffusion operator on graphs [10, 17] is defined as $\Delta_{ij} = A_{ij} - k_i\delta_{ij}$. Then, following [16], the diffusion equation on graph assumes the form

$$\frac{d\theta_i}{dt} = D\sum_j \Delta_{ij}\theta_j + \alpha f(\theta_i)\,. \tag{2}$$

where now D can be interpreted as the rate of the jump process between neighborhood sites, and θ_i is the field concentration at node i.

Now we can introduce some of our results on RD on graphs, studied with a discrete logistic reaction term $f(\theta_i) = \theta_i(1 - \theta_i)$ on network models representing realistic problems, characterized by two different structures of connections. Firstly there is the "short range" deterministic structure in which every node is connected to the nearest neighbors, $\forall\, i \in V$ $(i, i+1) \in E$ and $(i, i-1) \in E$. Secondly there is the "long range" random component in which many different connection between distant nodes start from a given subset of nodes, becoming hubs for the network. This is a crude model for the epidemiological diffusion dynamics inside infrastructures/transport network, or for the contact graph of the tertiary structure of proteins, in which one always has the local links forming the chain and long range links due to protein folding. More precisely we studied two

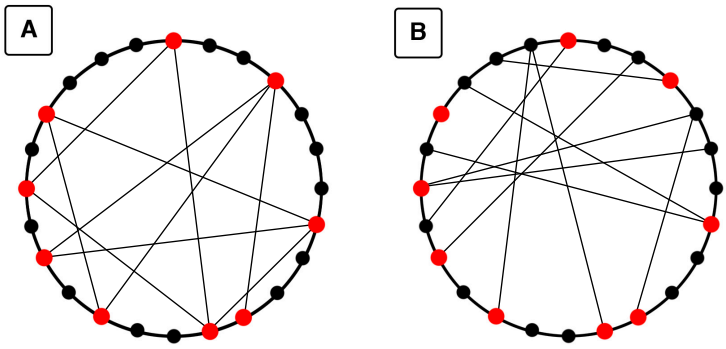

FIG. 1: A simple representation of the RenyiLike-Separable graph (A-graph, on the left) and the RenyiLike-Indivisible graph (B-graph, on the right). It should be noted that in the RenyiLike-Separable graph links starting from hubs end in other hubs, while in the RenyiLike-Indivisible graph links starting from hubs end in simple nodes.

different type of graphs, building long range links in two complementary ways: A-type have an Erdos-Renyi like structure among a subset of links chosen with probability p, and in B-type a subset of sites join long range connections with the other sites forming the graph with probability q, with $q = \frac{p(N-1)}{N_{tot}-N}$ to realted the two models, with respectively N_{tot} and N that are the number of sites of the graph and of the subset.

The first goal of our studies is to investigate the relation between the statistical topological properties of graphs with a large number of nodes, $O(10^5)$, and the dynamical behavior of RD process. In particular we are looking by a dynamical point of view to the filling time percentage $T(\Theta) = \min\{t \in R | M(t) \geq \Theta\}$, where $M(t) = \sum_i \theta_i(t)$. In the limit of mean-field dynamics, for $\alpha \ll 1$, the times needed to reach a percentage Θ of the filling can be easily computed from Eq. (**??**)

$$T_{mf}(\Theta) = \frac{1}{\alpha} \log \frac{\Theta(1 - M(0))}{M(0)(1 - \Theta)} \tag{3}$$

where $M(0)$ is the initial filling percentage. Therefore $T_{mf}(\Theta)$ is inversely proportional to α, while in the limiting case of a linear propagating front, for $\alpha \gg 1$, from Eq. (**??**) one has

$$T_l(\Theta) \sim \frac{\Theta}{v} \sim \frac{\Theta}{\sqrt{\alpha}}, \tag{4}$$

since $v \propto \sqrt{\alpha}$. To analyze topological properties we look at assortativity coefficient

$$r = \frac{L^{-1} \sum_i j_i k_i - \left[L^{-1} \sum_i \frac{1}{2}(j_i + k_i)\right]^2}{L^{-1} \sum_i \frac{1}{2}(j_i^2 + k_i^2) - \left[L^{-1} \sum_i \frac{1}{2}(j_i + k_i)\right]^2} \tag{5}$$

,where j_i and k_i are the degrees of the nodes at the ends of the ith edge, with $i = 1, \ldots, L$. Degree assortativity is the tendency inside the graph of sites with connectivity k_i to be connected to sites with the same degree k_i' (assortative network), or to sites with a straightly different connectivity (disassortative network).

Another important quantity is the average distance between two nodes

$$\langle l \rangle = \frac{1}{N_{tot}(N_{tot} - 1)} \sum_{ij} l_{ij} \tag{6}$$

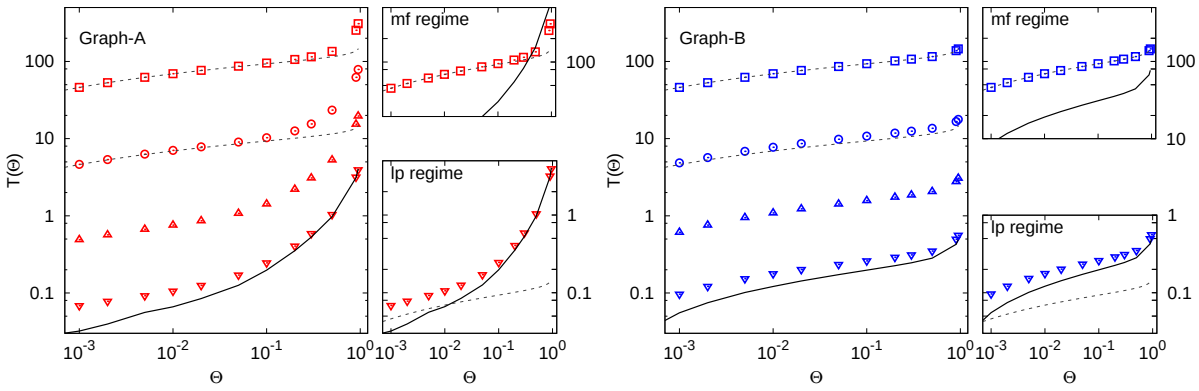

FIG. 2: Filling times, $T(\Theta)$, at varying filling percentages Θ for different values of α and setting $D = 1$ (from bottom to top $\alpha = 100$ ($\bigtriangledown$), $\alpha = 10$ ($\bigtriangleup$), $\alpha = 1$ ($\circ$), $\alpha = 0.1$ ($\square$)) for $p = 2p_c$ and both the case of RenyiLike-Separable graphs (Graph A, left, red) and RenyiLike-Indivisible graphs (Graph B, right, blue). Dashed and solid lines show the values of the filling times in the mean-field (Eq. (3)) and linear propagation in the graph topology (Eq. (11)) approximations, respectively. The panel "mf regime" stress for $\alpha = 0.1$ ($\square$) the goodness of the mean-field approximation together with the poor accuracy of the linear propagation approximation. The opposite is true for the panel "lp regime" where, for $\alpha = 100$ ($\bigtriangledown$), the goodness of the linear propagation approximation together with the poor accuracy of the mean-field approximation are highlighted.

where l_{ij} is the length of the minimal path connecting node i and node j, also known as the "chemical distance" between i and j.

Then we study the correlations between dynamical observables and statistical properties of the graph x, as

$$C(T(\Theta), x) = \frac{1}{n_s} \sum_{s=1}^{n_s} (T^s(\Theta) - T(\Theta))(x^s - x)/(\sigma_{T(\Theta)} \sigma_x) \tag{7}$$

among different realizations of the graph and of the dynamics $s = 1, ..., n_s$, where the quantities not related to a single realization s are averaged quantities, and σ the standard deviations. We have found that, although its widespread use [18], assortativity doesn't give predictive information on RD process on dual graphs. At the same time, we have found correlations between $\langle l \rangle$ and $T(\Theta)$, providing an interesting point of view to study transport problems on networks. This represents an evidence that the features of the reaction spreading on graphs is strictly related to the topological distance between nodes.

To exploit thoroughly such consideration, partially following ref [19], we introduce a partition of the graphs in sub-graphs, or rings, with the following property

$$R_i(l) = \{ j \in V \,|\, l_{ij} = l \}\,, \tag{8}$$

where i is the starting node of the reaction process: the ring $R_i(l)$ contains all the nodes whose minimum distance from the node i is l, and we set $R_i(0) = \{i\}$. Moreover we also define the cumulative ring as

$$G_i(l) = \cup_{\ell=0}^{l} R_i(\ell)\,. \tag{9}$$

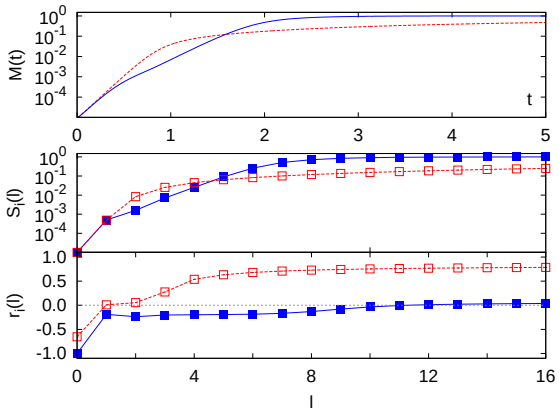

FIG. 3: Comparison between filling percentages as a function of time (top panel), and topological ring quantities (percentage of nodes up to the ring l, $S_i(l)$, middle figure, and ring assortativity up to the ring l, $r_i(l)$, bottom figure) as a function of l, in cases of RenyiLike-Separable graphs (red empty squares, dashed lines) and RenyiLike-Indivisible graphs (blue full squares, solid lines). The parameters used are $N_{tot} = 100000$, $N = 1000$ super connected sites, $\alpha = 10$, $D = 1$ and $p = 2p_c$.

In order to relate topological quantities such as $R_i(l)$ to the spreading dynamics we introduce $S_i(l)$ as the percentage of nodes of the graph contained within the ring $R_i(l)$:

$$S_i(l) = \frac{|G_i(l)|}{N_{tot}} = \frac{1}{N_{tot}} \sum_{\ell=0}^{l} |R_i(\ell)| \,, \tag{10}$$

where $|X|$ indicates the number of nodes in the set $X \subset V$. The quantity $S_l(l)$ is the maximum percentage of reaction products that can be contained within the ring $R_i(l)$.

In homogeneous media, the quantity of reaction products generated by the propagation of an FKPP front is proportional to the time and the filling time is given by Eq. (4), while when rewritten using the ring structure reads

$$T_i(l) = \frac{S_i(l)}{v_0} \tag{11}$$

where $T_i(l)$ is the filling time up to the ring l and $v_0 = 2\sqrt{D\alpha}$ is the front speed in the case of the simple FKPP model. In some sense Eq. (11) represents a standard FKPP front propagating in the graph topology.

We find that the degree of assortativity, that is considered the most relevant topological indicator to measure the spreading efficiency in reaction-diffusion problems on graphs, is only capable of giving some hints about the spreading process. We show that the most revealing topological quantity of the graphs, able to predict the features of the spreading process, is the percentage of links at minimum distance l from the initial node, $S_i(l)$(see Eq. (10)).

Next Steps

- In the context of RD dynamics in complex media, we are now investigating at the spreading and invasion problems on heterogenous media using an agent based approach for the trans-

port process and a mesoscopic coarse-grained approach for the reaction process, passing from PDE equations to stochastic processes. With this model it is possible to study fluctuation effects of RD process regarding discrete populations [20], very interesting from a biological point of view, where a populations made of a not large number of elements is involved. An example is the study of invasions from a biological reservoir to an heterogeneous habitat [21] studied with a PDE approach, also adding an advection term. The spreading process takes place in a periodic alternation of favorable and unfavorable patches, where the population die or grow, studying the conditions for successful invasions and the speed of the invasion process, in terms of patches sizes and advection speed. A step forward a realistic model of biological invasion in heterogeneous systems is to use models that take into account the discrete nature of biological population.

- Another interesting direction for my thesis is to make RD problem more realistic, using both different reacting terms $f(\theta)$ and network structures. For instance we can study epidemic diffusion in a city, using a network made of real transport infrastructures connections, like in the Global Mobility Network [22], and introducing RD epidemiological model, like SIR or SIS [23], where more than one field is involved. In the SIR model three different fields of concentration interplay in the process: susceptible, infectious and recovered concentrations interact in a system of paired RD equations. As we have done for autocatalytic reaction on graphs [24], in ref [22], exactly in the framework of the Global Mobility Network, the authors studied the relation between topological properties and dynamical observables, introducing an effective distance in networks looking at the statistical structure of connections (also for graphs with weighted connections), finding new metrics suitable to analyze spreading processes in different media. This approach can be analyzed more in depth and extended to different networks and reaction processes.

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