We study the two particle annihilation reaction $A + B \rightarrow \emptyset$ on interconnected scale free networks. We show that the mixing of particles and the evolution of the process are influenced by the number of interconnecting links and by their functional properties, while surprisingly when the interconnecting links have the same function as the links within the networks, they are not affected by the interconnectivity strategies in use. Due to the better mixing, which suppresses the segregation effect, we show that the reaction rates are faster than what was observed in other topologies, inline with previous studies performed on single scale free networks.

The use of complex networks to describe real systems of interacting entities is becoming standard practice [1, 2], but, currently the major challenge of network science is to understand how networks interact in an increasingly interconnected world. Networks in general retain their identity despite the existence of interconnections, for example a communication network does not change its role when it is connected to a power network. This makes our general knowledge about isolated networks still relevant for the interconnected case. But, some network properties are strongly affected by interconnectivity [3–10].

In addition, interconnecting links may be different (with respect to their function) than the normal links within the networks. In the example at hand, via interconnecting links we provide power to the communication network, and we control how the load is distributed in the power network. Thus, failure of these links has severe consequences, which is why in this case they are called dependency links [11]. In such cases extra care should be taken, and interconnected networks should not be studied as isolated networks with distinct communities. Indeed, recently it was shown that an interconnected system of networks may be either in a regime where the various networks are structurally independent, or in a regime where they are strongly coupled and the system behaves like one large network [12]. This can have a large influence on the evolution of dynamical processes on such systems.

In this work we provide a detailed numerical study of how interconnectivity affects the evolution of a diffusion-reaction dynamical process, when the reaction evolves on an interconnected network substrate. More precisely, we study the reaction rates of the annihilation reaction $A + B \rightarrow \emptyset$ on coupled Scale Free Networks (SFN) using different interconnecting strategies.
In SFN the probability to find a node with $k$ connections (degree) is given by $P(k) \sim k^{-\gamma}$. Such degree distributions allow the existence of a small number of nodes with very large number of links (i.e. hubs), while the majority of the nodes have only a few links. It is clear that the number of hubs depends on the value of the exponent $\gamma$, which typically has values in the range $2 < \gamma < 4$. Small values of $\gamma$ lead to heterogeneous networks, while as $\gamma$ increases, especially when $\gamma > 3$, the networks are getting more homogeneous.

The annihilation reaction $A + B \rightarrow \emptyset$, is an exemplary case of diffusion-controlled reactions which were used to model chemical reactions, epidemics, and other dynamical processes [13, 14]. In general, the quantity of interest is the concentration of particles $\rho(t)$ that remain in the system at a given time $t$, which follows

$$\frac{1}{\rho(t)} - \frac{1}{\rho_0} = \kappa t^f,$$

where $\rho_0$ is the initial particle concentration, and $\kappa$ is the rate constant. The maximum value of $f$ for various topologies is set by the mean-field asymptotic limit to $f = 1$, while the non-classical kinetics predict that the exponent $f$ depends on the dimensionality $d$ of the space where the process evolves as $f = d/d_c$ for $d \leq d_c$, and $f = 1$ for $d > d_c$ [15–19]. Here, $d_c$ is the upper critical dimension, which for the $A + B$ reaction is $d_c = 4$. Surprisingly, however, it was shown that when SFN are used as substrate $f$ can obtain values larger than one [20] and particles do not segregate, similar to what was observed in systems with Levy mixing [21].

This finding was based only on computer simulations, and showed a rapid acceleration of the process for networks with $\gamma \leq 3.5$. This acceleration was initially attributed to the existence of hubs, which affect the spatial distribution of particles. The spatial arrangement of particles at a given time $t$ was studied by the quotient $Q_{AB}(t)$, that measures how well-mixed the system is by comparing the number of contacts between particles of the same type ($N_{AA} + N_{BB}$) against the number of particles of different types ($N_{AB}$) [22]

$$Q_{AB}(t) = \frac{N_{AB}(t)}{N_{AA}(t) + N_{BB}(t)}.$$

Later, this process was treated analytically [23, 24], and subsequent publications tested the effect of the network generation mechanism on the reaction speed [25, 26].

Here we show that different to what was recently reported for other processes, like e.g. synchronization [10], the reaction rates of the annihilation reaction do not depend much on the interconnectivity strategy in use. Indeed, we show that the mixing of particles which determines the reaction rates depends mostly on the number of interconnecting links and their function, while the interconnectivity strategy plays only a marginal role.

The SFN used in our study have size $N \sim 10^5$ and are created using the standard configuration model [27–30] with $k_{\min} = 1$ following Ref. [20]. From the resulting network we extract and use
Figure 1: (a) Illustration of the three different interconnectivity strategies between two scale free networks. The CC strategy connects hub nodes from one network to hub nodes from the other network, while the PP strategy connects hub nodes from one network to peripheral nodes in the other network, and the CP strategy connects hub nodes from one network to peripheral nodes in the other. (b)–(d) The reaction progress $1/\rho - 1/\rho_0$ as a function of time for the three different interconnecting strategies of $n$-interconnections, applied on scale free networks with $\gamma = 2.5$, 3.0, and 3.5. With open symbols we present results for the “well mixed” case, while with dashed lines we present results for the “polarized” case. All networks had $N = 10^5$ nodes, the results are averaged over 100 realizations, and the standard errors are smaller than the size of the symbols. The continuous lines show the best fit at the asymptotic limit.

In order to create an interconnected system we use two networks generated with the above procedure, and add links between their nodes. The number $L$ of these interconnecting links is a fraction $q$ of the number of nodes $N$ that are available in each network, i.e. $L = qN$, and we allow only one interconnecting link per node. But, besides the mere number of interconnecting links, local properties of the interconnected nodes, like their degree $k_i$, can affect the global properties of the system of networks [10]. In order to test if (and how) degree-degree correlations between interconnected nodes affect the annihilation reaction’s evolution we use three distinct interconnectivity strategies, i) a central to central (CC) strategy that links the $L$ highest degree nodes of the two networks, ii) a peripheral to peripheral (PP) strategy that links the $L$ lowest degree nodes of the two networks, and iii) a central to peripheral (CP) strategy that links the $L$ highest degree nodes of one network to the $L$ lowest degree nodes of the second network. An illustration of these strategies is shown in Fig. 1(a).

Furthermore, interconnecting links can have different functions than the links within each network, so in this work we assume two distinct cases. The first case assumes that the interconnecting links have exactly the same properties and functions as the links within the networks, and we
call them \( n \)-interconnections. The second case assumes that the interconnecting links have an “immediate transport” property, and we call them \( t \)-interconnections.

In our setting, immediate transport means that when a particle during its diffusive motion in one network lands at a node that is linked to another network with a \( t \)-interconnection, then the particle is transferred to the interconnected node of the second network simultaneously. For example, with a \( t \)-interconnection we could represent a person that is active in two social networks and a particle could be a piece of information available to one network. When this information reaches this interconnected person, it immediately jumps and becomes available to the other social network.

We perform Monte Carlo simulations using networks with different exponents \( \gamma \), different \( q \) values, and different original configurations. Our results are averages of 100 realizations per configuration. For every realization a total number of \( M_0 = \rho_0 N \) particles are placed on randomly selected nodes. For simplicity we use equal population of particles \( A \) and \( B \), and we set \( \rho_0 = 0.5 \), so that in total half of the network’s nodes are populated initially. Furthermore, in order to understand the influence of this initial placement, we test two different configurations. The “well mixed” configuration, which allocates (randomly) half of the \( A \) and \( B \) particles to one network and half of them to the other, and the “polarized” configuration which places (randomly) all \( A \) particles to one network and all \( B \) particles to the other network.

This “polarized” configuration, is particularly interesting because it tests the mixing efficiency of the scale free topology in combination with the different interconnectivity strategies. In diffusion limited reactions, like the one studied here, improving the mixing efficiency is important as aggregation of particles can significantly slow down the reaction rates [16].

For our simulations we select an occupied node at random, together with one of its neighbouring nodes. If the neighboring node is empty, the particle moves and occupies a new position (diffusion phase). If the neighboring node is already occupied (reaction phase), then the particles annihilate if they are of different types, while if they are of the same type, nothing happens and the chosen particle remains at its original position. This procedure is repeated by continuously selecting, moving and (possibly) annihilating particles, until there are no particles left in the system. Due to the annihilation process the total number of particles \( M(t) \) is reduced with time. Thus, the time (in Monte Carlo Steps – MCS) required to update the system’s state is advanced inversely proportional to the current number of particles, by \( 1/M(t) \).

Here we would like to stress that additional care is taken for the treatment of interconnecting links. For the case of \( n \)-interconnections, the interconnecting link behaves like all other links, and the particle has the same probability to “jump” to the other network though the interconnecting

\[^{1}\text{We should note that in a more realistic setting this piece of information should also stay on the first network, while at the same time it “emerges” on the second one. But this is a modified reaction diffusion processes, and studying it is beyond the scope of our current work. However it is left for future study.}\]
link, as it has to follow any other link to neighboring nodes in the same network. But, for the case of \( t \)-interconnections things are different. More precisely, a \( t \)-interconnection is not considered during the diffusing motion of the particle, but only at the end when the particle has moved already. In this case, if the particle moves to a node that is \( t \)-interconnected then it is immediately transported to the other network. Also, after generating the initial configuration— and only for the case of \( t \)-interconnections— if there are interconnected nodes occupied by particles of different types, then these particles are annihilated immediately.

As shown in Figs. 1(b)-(c), for the case of \( n \)-interconnections and a well mixed system, our results are comparable to Ref. [20] for all different strategies. More precisely, the absence of kinetic effects seems to depend more on the exponent \( \gamma \) than on the strategy we use to interconnect the nodes. For example, for the CC strategy we find \( f = 1.7 \pm 0.02 \) for \( \gamma = 2.5 \), \( f = 1.25 \pm 0.01 \) for \( \gamma = 3.0 \), and \( f = 1.14 \pm 0.01 \) for \( \gamma = 3.5 \). However, if we focus on a specific exponent, e.g. \( \gamma = 3.0 \), then...
Figure 3: (a) The reaction progress $1/\rho - 1/\rho_0$ for the “polarized” case as a function of time, evolving on two coupled scale free networks with $\gamma = 3.0$, and $n$-interconnections. The fraction of interconnecting links is $q = 0.1$ arranged according to the CC (circle), CP (triangle), and PP (square) strategy. (b) Same as previous, for $t$-interconnections. (c) The ratio $Q_{AB}$ over time for $n$-interconnections, and (d) for $t$-interconnections. All networks had $N = 10^5$ nodes, the results are averaged over 100 realizations, and the standard errors are smaller than the size of the symbols. The continuous lines in (a) and (b) show the $1/\rho \sim t$ behavior, and the dashed line at $Q_{AB} = 1$ in (c) and (d) corresponds to perfect mixing.

we find for $f = 1.24 \pm 0.01$ for CC, $f = 1.26 \pm 0.01$ for CP, and $f = 1.28 \pm 0.01$ for PP. This shows that an interconnected system of two SFN with $n$-interconnections behaves like one large SFN for a reaction-diffusion process. Also, the same asymptotic behavior holds even when the system starts from a completely polarized configuration. Of course, as expected, initially in this case the reaction rates are small, but, as time advances the system becomes better mixed and the reaction happens much faster. This essentially shows that the presence of a scale free topology alone, contributes to the mixing of particles, and enhances desegregation.

This is better visible in Fig. 2(a), where the mean-field predicted limiting case $1/\rho \sim t$ is included. When viewed together with Fig. 2(c), it becomes clear that the different strategies do not really affect the mixing of particles, and as a consequence the reaction rates. However, while even with the use of $t$-interconnections we obtain similar findings with respect to the reaction rates, as shown in Fig. 2(b), the CC strategy is now more effective in particle mixing, at least in
Figure 4: (a) The reaction progress $1/\rho - 1/\rho_0$ for the “well mixed” case as a function of time, evolving on two coupled SFN with $\gamma = 3.0$, and fraction of $n$-interconnecting links $q = 0.1, 0.2$, and 0.5, arranged using a CC strategy. (b) Same as previous, for $t$-interconnecting links. (c) The ratio $Q_{AB}$ over time for the $n$-interconnecting links, and (d) for the $t$-interconnection links. All networks had $N = 10^5$ nodes, the results are averaged over 100 realizations, and the standard errors are smaller than the size of the symbols. The continuous lines in (a) and (b) show the $1/\rho \sim t$ behavior, and the dashed line at $Q_{AB} = 1$ in (c) and (d) corresponds to perfect mixing.

Intermediate time scales, as shown in Fig. 2(d).

This attribute of the CC strategy is more pronounced when we start with an extremely polarized case, as shown in Fig. 3. More precisely, while the overall mixing and reaction rates are similar in the case of $n$-interconnections (see Figs. 3(a) & 3(c)), the better mixing achieved by the CC strategy is clear in the presence of $t$-interconnections. In this case, as shown in Figs. 3(b) & 3(d), the $Q_{AB}$ values for CC are higher at all times, and the concentration of the particles decreases much faster. However, at longer times the mixing achieved by the other strategies improves, while at the same time the number of particles decreases. This leads to a crossover point around $t = 11$ MCS where the reaction rates increase rapidly, as shown by the values of $f$ (i.e. $f = 1.44 \pm 0.02$ for CC, $f = 1.57 \pm 0.02$ for CP, and $f = 1.69 \pm 0.05$ for PP) that converge to a similar asymptotic behavior for all three strategies (Fig. 3(b)).

Similar observations are made for different $q$ values as shown in Figs. 4 and 5. In this case it is
Figure 5: (a) The reaction progress $1/\rho - 1/\rho_0$ for the “polarized” case as a function of time, evolving on two coupled SFN with $\gamma = 3.0$, and fraction of $n$-interconnecting links $q = 0.1, 0.2,$ and 0.5, arranged using a CC strategy. (b) Same as previous, for $t$-interconnecting links. (c) The ratio $Q_{AB}$ over time for the $n$-interconnecting links, (d) for the $t$-interconnection links. All networks had $N = 10^5$ nodes, the results are averaged over 100 realizations, and the standard errors are smaller than the size of the symbols. The continuous lines in (a) and (b) show the $1/\rho \sim t$ behavior, and the dashed line at $Q_{AB} = 1$ in (c) and (d) corresponds to perfect mixing.

It is easier to see that higher $q$ values result to better mixing of particles, as expected since the system becomes better connected. In addition, the mixing is enhanced much more by the presence of $t$-interconnections, as shown by comparing Fig. 4(c) to Fig. 4(d), and Fig. 5(c) to Fig. 5(d). However, the same conclusions are true with respect to the increasing of the reaction rates at longer times, which allows the convergence to the same asymptotic behavior.

Summarizing, we studied the annihilation reaction $A + B \rightarrow \emptyset$ in interconnected SFN, when different interconnectivity strategies are used, and when the interconnecting links have different functionality than the normal links. We find that the system of networks exhibit rapid reaction rates, in line with a previous observation about single SFN [20] – which is different from what was observed in other topologies, like lattices and fractals. In addition, different from what was reported for other processes where, for example, in the presence of $n$-interconnections CC is the best strategy to achieve synchronization [10], here we showed that the function and the number of
interconnecting links plays more important role than the interconnection strategy to the mixing of particles. We thus identified ways to suppress the segregation phenomenon and enhance the diffusion of particles. Besides their relevance to reaction kinetics, our findings could be applied to model propagation of conflicting information in social networks, and highlight ways to reduce polarization.

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