1. Introduction

1.1. General motivation

Nowadays it is widely accepted that the functioning of complex systems [1] depends on dynamical processes taking place between the interacting entities of networked structures, which are well described by mathematical models based on discrete systems, such as graphs and networks [2-5]. Diffusion is a ubiquitous physical driver of many of these dynamics, ranging from the flow of information in social networks, transport in infrastructural systems, epidemic spreading processes, and the synchronization of biological, social or technological entities [6-8]. A general assumption of the diffusive dynamics on discrete systems is conservativeness. That is, it is assumed that the total amount of diffusing items is conserved along the time at the entities of the system. For instance, let us consider an intercellular proximity network $G=(V,E)$ (see [9]) in which the vertices $j\in V$ represent cells in an epithelium tissue and its edges represent the proximity (via a Voronoi diagram) between cells (see **Fig. 1** (a)). It is well known that ions and large molecules diffuse rather freely from one epithelial cell to another [10] but does not diffuse along the intercellular space to the exterior. This is because the permeability of the junctional surfaces of the cell membranes is very high, but the nonjunctional surfaces and intercellular spaces represent strong diffusion barriers. If we represent the concentration of ions/molecules on the epithelial cells (vertices of the graph) at initial time to be the column vector $\boldsymbol{u}_0$, the conservativeness of the process is expressed by the fact that $\mathbf{1}^T\boldsymbol{u}(t) = \mathbf{1}^T\boldsymbol{u}_0$, for any time t, where $\boldsymbol{u}(t)$ is the vector of concentrations at the nodes of the graph at time t and $\mathbf{1}$ is a column vector of ones.

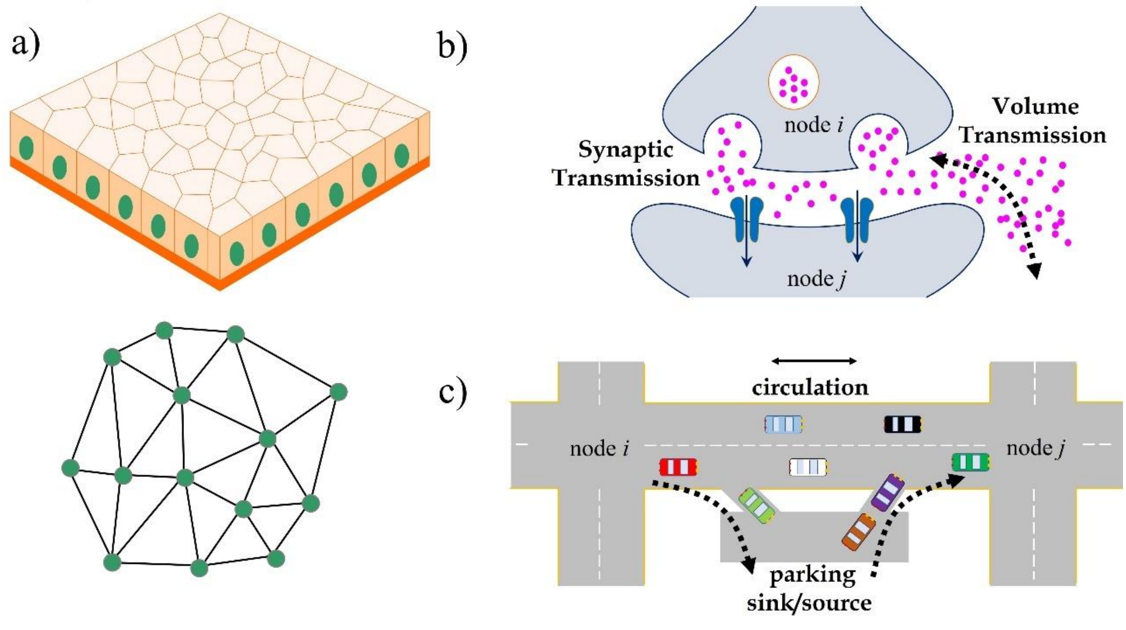


Fig. 1. (a) Illustration a portion of epithelial tissue (top panel) and its graph representation (bottom panel), where the conservative diffusion of ions and molecules occur. (b) Example of nonconservative dynamics consisting of neurotransmitters (NT) being spilled over between two neurons due to the so-called volume transmission through the extracellular milieu. (c) The nonconservative traffic flow of cars in a city where the number of cars at intersection A is not necessarily the same as those at intersection B due to the emergence/sinking of cars from parking spaces.

The same assumption can be assumed (and it is typically assumed (see for instance [11])) for the synaptic interaction between two neurons. However, this is not necessarily the case for the chemical synapses where the so-called volume transmission (VT) is well-documented [12-16]. In this case some concentrations of neurotransmitter are spilled over the extracellular fluid filling channels of the extracellular space and the cerebrospinal fluid filling ventricular space and sub-arachnoidal space (**Fig. 1** (b)). Then, it is no longer true that $\mathbf{1}^T \boldsymbol{u}(t) = \mathbf{1}^T \boldsymbol{u}_0$, and the process is nonconservative. Another example of nonconservative diffusion occurs when urban traffic is accounted by the number of cars flowing from the intersections of an urban street network as illustrated in **Fig. 1** (c). The no-conservativeness of this diffusion surges from the fact that cars may emerge/disappear due to parking spaces located at street legs. More examples of nonconservative diffusion include the communication in social media [17-19] like Twitter where a user can post a message who can be read by her followers, but also (if not constrained by the user) by non-followers, all of whom can retweet such information to others. Also, in a food web [20] when one species A (predator) predates another species B (prey) there is a mass transfer from B to A, but if A utilizes only a portion of the material and free energy originally in B, which is then retained in the predator, the resulting process is a non-conservative one. Such mass and energy can then be diffused across the food web in a non-conservative diffusive way.

The qualitative differences between conservative and nonconservative diffusion are schematically represented in **Fig. 2** where N_t is the total number of particles at the vertices of the graph at time t.

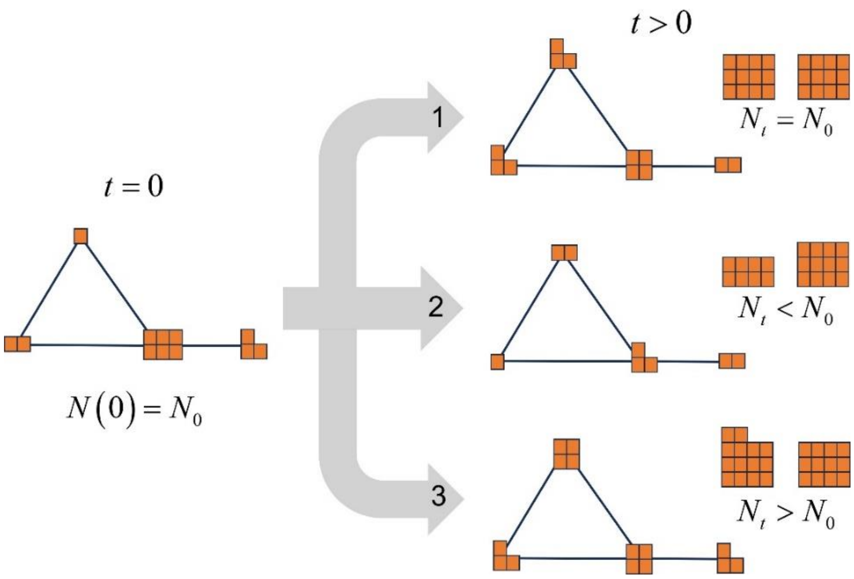


Fig. 2. Differences between conservative (1) and nonconservative (2 and 3) diffusive processes in a graph.

1.2. Nonconservative (NC) diffusion on graphs

Conservative diffusion is described by the “classical” diffusion equation: $\dot{\boldsymbol{u}}(t) = -L\boldsymbol{u}(t)$ [4, 21], with initial condition $\boldsymbol{u}(0) = \boldsymbol{u}_0$, where L is the standard graph Laplacian (see later for definition). Its time evolution is characterized by the existence of a steady state in which $\boldsymbol{u}(t \to \infty) = \frac{1}{n(\mathbf{1}^T \boldsymbol{u}_0)}$. That is, the state of the nodes converges to the average of their initial states in a consensual way (see **Fig. 3** top-left panel).

A direct consequence of the fact that $\mathbf{1}^T\boldsymbol{u}(t) \neq \mathbf{1}^T\boldsymbol{u}_0$ in a nonconservative diffusion is that the system does not reach a steady state in which $\boldsymbol{u}(t \to \infty) = \frac{1}{n(\mathbf{1}^T\boldsymbol{u}_0)}$, but instead the states of the nodes can diverge (**Fig. 3** top-right panel), stabilize at certain values which are smaller than the initial ones (**Fig. 3** bottom-left panel) or vanish (**Fig. 3** bottom-right panel).

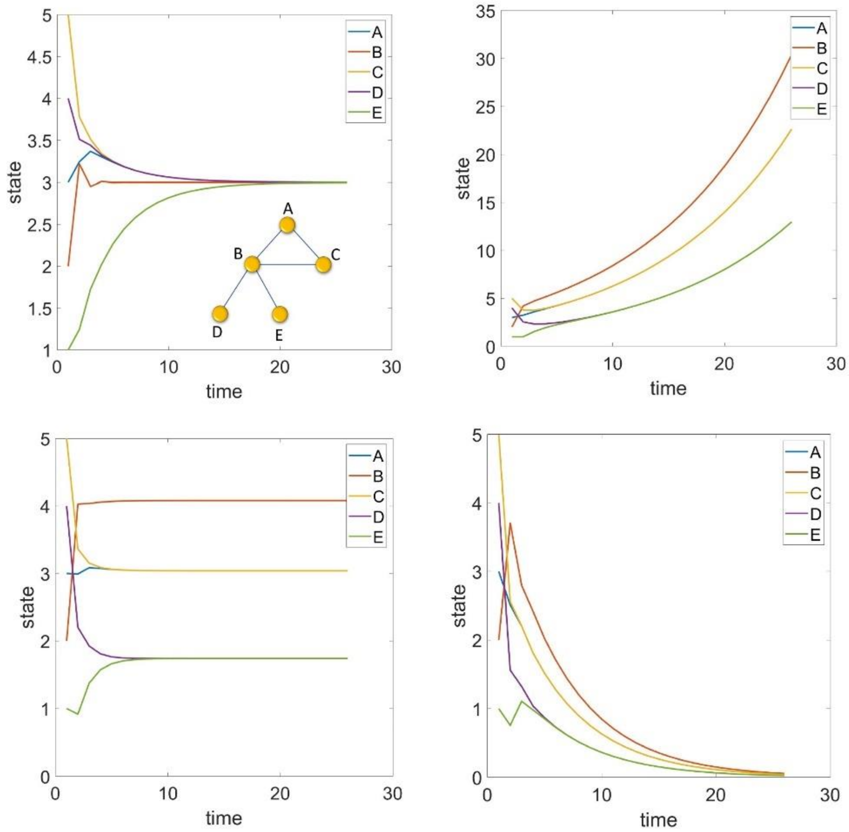


Fig. 3. Differences in the time evolution of a conservative (top-left) and nonconservative (the three other panels) diffusive processes in a network.

A way to describe NC diffusion on graphs is by considering $\dot{\boldsymbol{u}}(t) = -L_\chi\boldsymbol{u}(t)$, with initial condition $\boldsymbol{u}(0) = \boldsymbol{u}_0$, where $L_\chi \coloneqq \chi I - A$ is the Lerman-Ghosh Laplacian [22] of the graph, where $\chi \geq 0$ is an empirical parameter. Then, we can prove the following.

Lemma 1. Let $\dot{\boldsymbol{u}}(t) = -L_\chi\boldsymbol{u}(t)$, $\boldsymbol{u}(0) = \boldsymbol{u}_0$, where $L_\chi \coloneqq \chi I - A$, and let $\lambda_1 > \lambda_2 \geq \cdots \geq \lambda_n$ be the eigenvalues of A for a connected, simple graph. Then,

$$\lim_{t\to\infty} \boldsymbol{u}(t) = \begin{cases} (\boldsymbol{\psi}_1^T\boldsymbol{u}_0)\boldsymbol{\psi}_1 e^{t(\lambda_1-\chi)} = \infty & \text{for } \chi < \lambda_1, \\ \left(\boldsymbol{\psi}_1 \sum_j u_0(j)\psi_1(j)\right) & \text{for } \chi = \lambda_1, \\ (\boldsymbol{\psi}_1^T\boldsymbol{u}_0)\boldsymbol{\psi}_1 e^{-t(\chi-\lambda_1)} = 0 & \text{for } \chi > \lambda_1. \end{cases}$$

The case when $\chi = \lambda_1$ is a very specific one and its solution is trivial, and the final state depends on the so-called eigenvector centrality of the graph. The case when $\chi < \lambda_1$ seems unrealistic from a real-world perspective as the "concentration" of items at the vertices of the graph growth to infinite. The last case, when $\chi > \lambda_1$, may represent some realistic scenarios in which the vertices of a graph get empty by discharging their content to the environment. However, these three scenarios do not describe realistically cases of interest from a complex systems perspective like the ones mentioned before, i.e., volume transmission in synapses, urban traffic, diffusion of information via social media, etc.

Therefore, in this section of the project we propose to consider reaction-diffusion models, where we allow that the vertices create or annihilate items to avoid that their concentrations go to zero or to infinity:

$$\dot{\boldsymbol{u}}(t) = -L_{\chi}\boldsymbol{u}(t) + f\big(\boldsymbol{u}(t)\big).$$

Then, although the diffusive dynamics considered by the previous equation is non-conservative, it reaches a steady state in which the concentration at every vertex in the graph is the same as illustrated in the **Fig. 4**. The details of this part of the project are given in the next section.

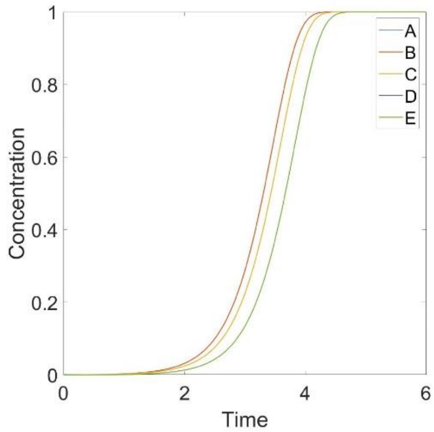


Fig. 4. Illustration of the time evolution of a NC process controlled by a reaction-diffusion model where the concentration of items at the vertices of the graph (the same as in **Fig. 3**) reach a steady state.

1.3. Spatial nonlocality in NC diffusion

There are complex system scenarios in which the diffusion of items occurs not only via the interaction among nearest neighbours. One example is provided by the volume transmission of NT among neurons during synapses [13-16]. The volume transmission (VT) has been defined as [13] *"a diffuse mode of intercellular communication affecting and modulating the activity of entire brain regions"*. This mode of diffusion differs significantly from the wiring transmission where there is [13] "*a virtual wire connecting the cell source of the signal (message) with the cell target of the signal."* In the VT, a NT can be spilled over from one neuron, then navigate via blood vessels or the cerebrospinal fluid and being recaptured by a target neuron which is not wirily connected with the source of this transmission (see **Fig. 5**). From the perspective of the vertices of a graph what happen in this process is the following. Items located at a given vertex i of the graph are spilled over outside the graph like in any nonconservative process. Then, these items are not only recaptured at the nearest neighbors of vertex i (the nonconservative process described in the previous subsection), but also by vertices which are at certain topological distance from it (a spatial nonlocal process).

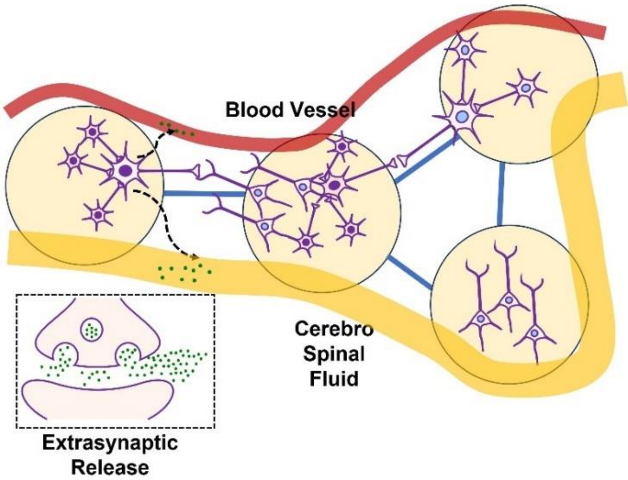


Fig. 5. Illustration of the volume transmission of NT via blood vessels and/or cerebrospinal fluid between distant neurons.

A realistic assumption for these spatial nonlocal processes is to consider that the chances of an item to hop from one vertex i to another vertex j of the graph decays with the topological separation between the two vertices. In the case of urban traffic, for instance, standard diffusive models assume that cars stop at every intersection, which correspond to hopping between nearest neighbour vertices of the urban street network. A nonlocal approach to this dynamic will assume that cars not necessarily stop at every intersection but that can go two, three, etc., streets without stopping with chances of going too far without stopping being heavily penalized. Other scenarios, like the diffusion of information through social media can also easily adapted to this general scenario.

In the case of conservative diffusion there are two approaches to describe these spatial nonlocal processes on graphs. On one hand, our group has generalised the concept of graph Laplacian by introducing the d-path Laplacians [23-26], which captures long-distance hops in graphs. By means of the transformation (Mellin, Laplace, etc.) of these operators we modulate the decay of the chances of hopping between vertices at given topological distance. On the other hand, physicists Riascos and Mateos [27, 28] proposed the use of fractional powers of the graph Laplacian, which is a positive-semidefinite matrix as a spatial nonlocal operator. For a comparison of both approaches see [29].

In this section of the project, we propose to introduce spatial nonlocal effects on NC diffusion on graphs. We will consider the case of dynamics described by: $\dot{\boldsymbol{u}}(t) = -\tilde{L}_{\chi}\boldsymbol{u}(t)$, for the sake of generality, but we will mainly focus on the study of the reaction-diffusion models of the type: $\dot{\boldsymbol{u}}(t) = -\tilde{L}_{\chi}\boldsymbol{u}(t) + f(\boldsymbol{u}(t))$. Here, $\tilde{L}_{\chi}$ represents the transformed d-path Lerman-Ghosh Laplacian of the graph, which will be formally defined in this project, e.g., $\tilde{L}_{\chi} \coloneqq \sum_{d=1}^{diam} d^{-s}(\chi I - A_d)$, where A_d are the d-path adjacency operators (see further). The fact that L_{χ} may not be positive (semi)definite, for instance when $\chi < \lambda_1(A)$, the fractional powers of this matrix may not exist, may not be unique in case of existing, and are complex when they exist. This invalidates the possibilities of using Riascos-Mateos approach of fractional powers of the NC Laplacian and left only the possibility of extending the NC Laplacian of Lerman-Ghosh to cases of d-path NC Laplacians and their transformations, which will be the focus of this section of the project.

1.4. Temporal nonlocality in NC diffusion

A characteristic feature of complex systems is the existence of certain memory about the past. That is when we consider the time evolution of the NC diffusion: $\dot{\boldsymbol{u}}(t) = -L_\chi \boldsymbol{u}(t)$, $\boldsymbol{u}(0) = \boldsymbol{u}_0$ at the time instant a we simply do not consider the temporal trajectory of $\dot{\boldsymbol{u}}(t < a)$. That is, we consider that the system has no memory about its part. A way to introduce the memory of the system about past is to consider a weighted sum of the values of $\dot{\boldsymbol{u}}(t \leq a)$ such that we give more weight to the present, i.e., $t = a$, than to the past, $t < a$. This is schematically represented in **Fig. 6** (see [30]), where the weighted sum is replaced by the integral from time 0 to a, of the product of $\dot{\boldsymbol{u}}(t)$ and the weights $\vartheta(t)$, which increases as $t \rightarrow a$.

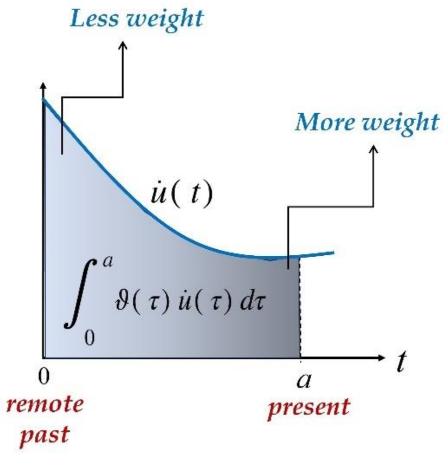


Fig. 6. Illustration of consideration of “memory” in the temporal evolution of a dynamics.

In this section of the project, we will consider the replacement of the memoryless derivative $\dot{\boldsymbol{u}}(t)$ by the fractional Caputo derivative [31-33],

$$D_t^\alpha \boldsymbol{u}(t) := \begin{cases} \dfrac{1}{\Gamma(1-\alpha)} \displaystyle\int_0^t \dfrac{\dot{\boldsymbol{u}}(\tau) d\tau}{(t-\tau)^\alpha} & 0 < \alpha < 1, \\ \dot{u}(\tau) & \alpha = 1, \end{cases}$$

where $\vartheta(t) = \frac{1}{\Gamma(1-\alpha)(t-\tau)^\alpha}$.

Therefore, our focus in this section is the study of the temporal nonlocal NC diffusion equations of the type:

$$D_t^\alpha \boldsymbol{u}(t) = -L_\chi \boldsymbol{u}(t) + f\big(\boldsymbol{u}(t)\big), \boldsymbol{u}(0) = \boldsymbol{u}_0,$$

with and without the reactive part, $f\big(\boldsymbol{u}(t)\big)$.

In particular, we will investigate the solutions of these equations in terms of the Mittag-Leffler matrix functions [34, 35] of L_χ:

$$E_\alpha(L_\chi) := \sum_{k=0}^{\infty} \frac{(L_\chi)^k}{\Gamma(\alpha k + 1)}$$

where Γ is the Euler gamma function.

1.5. Time-and-space nonlocal NC diffusion

In the case of conservative diffusion, we have previously considered a generalised model that accounts simultaneously for time and space nonlocal effects [36]:

$$D_t^{\alpha}\boldsymbol{u}(t) = -\left(\sum_{d=1}^{diam} d^{-s} L_d\right)\boldsymbol{u}(t), \qquad \boldsymbol{u}(0) = \boldsymbol{u}_0,$$

where d is the shortest path distance between pairs of vertices, $s > 0$ is the strength of the long-range jumps and L_d is the d-path Laplacian matrix. Using this model, we have proved that the conservative diffusion on graphs can give rise to sub-diffusive, normal and super-diffusive behaviour depending on the parameters s and α selected for a given type of graph as illustrated schematically in **Fig. 7**.

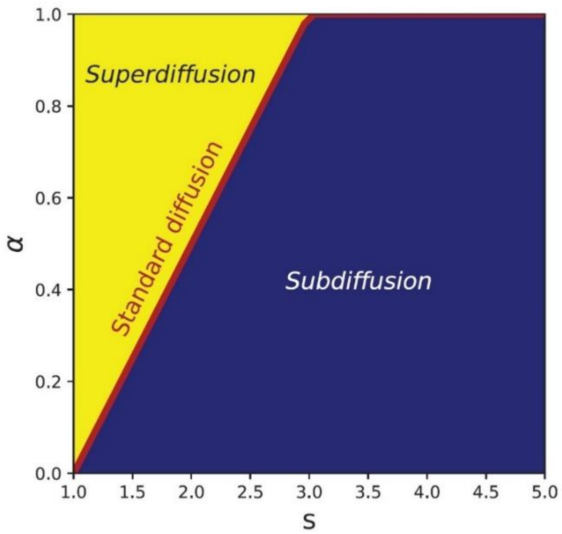


Fig. 7. Schematic representation of the different kinds of diffusion that emerge on a graph with the time-and-space generalised conservative diffusion model.

Therefore, tis part of the project will consist of the generalization of the NC diffusion equation to account simultaneously for time (through the time-fractional Caputo derivative) and space (through the transformed d-path Lerman-Ghosh Laplacians):

$$D_t^{\alpha}\boldsymbol{u}(t) = -\tilde{L}_{\chi}\boldsymbol{u}(t) + f\big(\boldsymbol{u}(t)\big), \boldsymbol{u}(0) = \boldsymbol{u}_0.$$

We will consider the purely diffusive process, i.e., without $f\big(\boldsymbol{u}(t)\big)$, and with such term. In the first case, we are interested in the analysis of the solution:

$$\boldsymbol{u}(t) = -E_{\alpha}\big(\tilde{L}_{\chi}\big)\,\boldsymbol{u}_0,$$

and the determination of conditions for anomalous diffusion (sub- and super-diffusion), if they exist. In the case of reaction-diffusion models we will consider a logistic model (see further) whose solution is expressible in terms of the two-parameters Mittag-Leffler function:

$$E_{\alpha,\beta}\big(\tilde{L}_{\chi}\big) \coloneqq \sum_{k=0}^{\infty} \frac{\left(\sum_{d=1}^{diam} d^{-s}(\chi I - A_d)\right)^k}{\Gamma(\alpha k + \beta)},$$

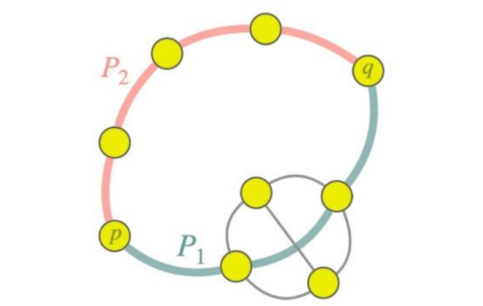
where we will be again interested in the analysis of the diffusive processes giving rise in terms of the parameters s and α.

1.6. Geometry of nonlocal NC diffusion

An important and desirable characteristic of the analysis of diffusive models on graphs/networks is to detect the most probable trajectories of the diffusive particles across the vertices and edges of G. For long time it was assumed that "information" flows through shortest (topological) paths in systems like the brain (see for instance [37]), where the lack of global information about its global structure makes such navigation impossible. Nowadays, alternative ways of navigation are studied for the communication between different vertices of networks, particularly in brain networks [38-40]. The topic is not new, think for instance on the effective resistance of an electrical network [41], which was proved 20 years ago to be a squared Euclidean distance between the vertices of a graph [42]. The resistance distance is directly related to the commute time of a random walker navigating the graph [43-45], which make it an attractive metric. Unfortunately, as proved by von Luxburg et al. [46], in large graphs, commute distance converges to an expression that does not consider the structure of the graph at all and that it is completely meaningless as a distance function on the graph.

Once a distance is defined on the graph it is possible to find the geodesic paths connecting pairs of vertices based on it [47, 48]. In this way we can, for instance, obtain the most probable trajectory of a random walker navigating between two vertices of the graph via a graph geometrization based on the resistance distance. In the last ten years our group has developed a new circum-Euclidean distance between the pairs of vertices of a graph known as the communicability distance [49-57], which allows to detect the shortest communicability paths in a graph, i.e., the most probable paths used by particles in a NC diffusion on the graph (see [55, 58]). Let us define the hitting time as the time (number of steps) that a random walker, departing from p, takes to hit by the first time the node q and the excess time as the time (number of steps) taken by a random walker, departing from p, to arrive at q in comparison with a ballistic walk. Then, if we consider the graph illustrated in **Fig. 8**, we can see that the shortest topological path (P_1) is not the most probable trajectory for a random walker as provided by the hitting and excess times. In this case, P_1 is also the shortest resistance path. However, the shortest communicability path coincides with the one having the least excess and hitting times. These results have been confirmed for a real-world network representing 638 brain regions in humans in which the communicability shortest paths have always provided least excess time than the shortest topological one [58].

Therefore, in this section of the project our focus will be in extending the concept communicability distance and communicability shortest paths to the cases in which the NC diffusion considers time-and-space nonlocal effects. This implies that we will extend the definition of communicability distance to other matrix functions beyond the exponential, i.e., Mittag-Leffler matrix functions, as well as beyond the simple adjacency matrix to consider matrices of the form: $\sum_{d=1}^{diam} d^{-s} A_d$ as will be described further in this project.



	P_1	P_2
Excess time	2.7	1.38
Hitting time	10.9	6.9
Shortest topological path	3	4
Shortest resistance path	2.15	3.38
Shortest communicability path	5.09	4.80

Fig. 8. A simple graph in which two different paths (P_1 and P_2) between the vertices p and q are considered. We give the values of the excess and hitting times between the two vertices after 1,000 random realizations. Additionally, we report the values of the length of the shortest topological, resistance and communicability paths.

2. OBJECTIVES

2.1. General

The main goal of this project is to develop a general mathematical theory for the study of NC diffusion dynamics on graphs/networks. Although NC diffusion has been previously studied on graphs it has not been sufficiently developed as to occupy the important place it should have in the analysis of complex systems. This general goal will be fulfilled by studying a reaction-diffusion logistic model on graphs. Although this dynamic is NC, it reaches an equilibrium steady state in which the concentration of items at the nodes neither diverges nor vanishes. We will then generalise these NC diffusion models to account for time-and-space nonlocal effects. The spatial nonlocality will be introduced by means of a generalisation of the adjacency operator of graphs to transformed d-path adjacency operators. Such transformations will be implemented to account for the decay of spatial nonlocality with the inter-vertex separation in the graph. The temporal nonlocality will be implemented by replacing standard derivatives by time-fractional Caputo derivatives in the NC diffusive models. Finally, we will also consider the geometries induced by these nonlocal NC diffusion dynamics and analyse the most probable trajectories of diffusive particles via geometrization of the graphs. As a general objective we will focus on integrating all these results for the analysis of small graphs, as well as large real-world networks.

2.2. Specific objectives

i. Propose a reaction-diffusion logistic model on graphs, finds analytically its exact solution and propose bounds to it, which allow its approximate solution for graphs and networks of relatively large sizes;

ii. Implementing spatial non-local interactions on NC diffusion on graphs. Studying the main mathematical properties of these generalised operators in (one-dimensional) infinite graphs, i.e., self-adjointness, boundness. Studying analytically the existence or not of super-diffusive behaviour for transforms (Laplace, factorial and Mellin) of these generalised operators in one-dimensional infinite graphs. Studying the main characteristics of the spatially nonlocal NC diffusive processes on real-world networks using these generalised operators;

iii. Implementing temporal non-local interactions on NC diffusion on graphs via Caputo fractional derivative. Studying the main mathematical properties of the solution of this model to check the existence or not of sub-diffusive behaviour. Studying the main characteristics of the temporal nonlocal NC diffusive processes on real-world networks using these generalised operators;

iv. Generalising the NC diffusive model to account simultaneously for time-and-space nonlocality. Finding general conditions for the existence of normal, sub- and super-diffusion on graphs under this model, and studying it in realistic networked scenarios;

v. Defining and analysing the geometries induced by the time-propagation operators generated in the solution of the time-and-space nonlocal NC diffusion models. Studying the general properties of the induced embedding, i.e., circum-Euclideanness, as well as defining and studying parameters like distances, angles spanned by position vectors, etc.;

vi. Defining and analysing the most probable “trajectories” of items when diffusing non-conservatively and nonlocally on a graph by means of geometrizations of the graphs based on the previously defined metrics;

vii. Integrate the previous objectives into a generalised theoretical framework in which the NC diffusion plays a central role in dynamical processes on complex systems.

3. METHODOLOGY AND WORKING PLAN

Let $G = (V, E)$ be a simple, undirected graph. Let $\mathcal{H} \coloneqq \ell^2(V)$ be the Hilbert space of square-summable functions on V and let $f \in \mathcal{H}$ be a function. Then [59, 60],

$$(\mathcal{A}f)(v) \coloneqq \sum_{w \in V:\,(v,w) \in E} f(w),$$

is the adjacency operator of G. If G is an infinite locally finite graph then $\mathcal{A}$ is a bounded selfadjoint operator on $\mathcal{H}$. The degree operator on G is defined as

$$(\mathcal{K}f)(v) \coloneqq k_v f(v),$$

where k_v is the degree of v. The Laplacian operator on G is defined as [59, 60],

$$(\mathcal{L}f)(v) \coloneqq \sum_{w \in V:\,(v,w) \in E} \big(f(v) - f(w)\big),$$

which is a bounded selfadjoint operator on $\mathcal{H}$ when the graph is infinite and locally finite. In finite graphs the three operators are realised by the corresponding adjacency, degree and Laplacian matrices: A, K, L. The Laplacian operator can be expressed as

$$(\mathcal{L}f)(v) = (\mathcal{K}f)(v) - (\mathcal{A}f)(v),$$

which in matrix form is: $L = K - A$.

In 2012 Lerman and Ghosh [22] proposed the following Laplacian matrix for a graph: : $L_\chi = \chi I - A$, where I is the identity matrix and $\chi \geq 0$ is an empirical parameter. We can write this matrix in operator form as

$$\big(\mathcal{L}_\chi f\big)(v) = \sum_{w \in V:\,(v,w) \in E} \left(\frac{\chi}{k_v} f(v) - f(w)\right).$$

The Abstract Cauchy Problem for the diffusion of potentials on the graph G is expressed by

$$\frac{d\boldsymbol{u}(t)}{dt} = \dot{\boldsymbol{u}}(t) = -\mathcal{M}\boldsymbol{u}(t), \qquad \boldsymbol{u}(0) = \boldsymbol{u}_0,$$

where $\mathcal{M}$ is either L or L_χ, $\boldsymbol{u}(t)$ is the vector of potentials, e.g., concentrations, densities, opinions, etc.

The conservative nature of the process $\dot{\boldsymbol{u}}(t) = -L\boldsymbol{u}(t)$ can be proved by considering its solution: $\boldsymbol{u}(t) = e^{-tL}\boldsymbol{u}_0$, and taking its Taylor series expansion: $\mathbf{1}^T\boldsymbol{u}(t) = \mathbf{1}^T e^{-tL}\boldsymbol{u}_0 = \mathbf{1}^T\boldsymbol{u}_0 - t\mathbf{1}^T L\boldsymbol{u}_0 + \frac{t^2}{2!}\mathbf{1}^T L^2\boldsymbol{u}_0 + \cdots$. Then, because L is positive semidefinite, $\mathbf{1}^T L = 0$ and so $(\mathbf{1}^T L)L^{k-1} = 0$. Thus, $\mathbf{1}^T\boldsymbol{u}(t) = \mathbf{1}^T\boldsymbol{u}_0$ for any t. The nonconservativeness of the process $\dot{\boldsymbol{u}}(t) = -L_\chi\boldsymbol{u}(t)$ is proved by **Lemma 1**. Notice that this process may be conservative only in the special case when $\chi = \lambda_1$ and $\boldsymbol{u}_0 = \boldsymbol{\psi}_1$.

3.1. Logistic NC diffusion on graphs/networks

Participants: Ernesto Estrada (IFISC), PhD candidate

In this section of the project we propose the study of the following reaction-diffusion model with NC diffusion as controlled by the Lerman-Ghosh Laplacian:

$$\dot{\boldsymbol{u}}(t) = -\gamma L_{\chi}\boldsymbol{u}(t) + f(\boldsymbol{u}(t)), \quad \boldsymbol{u}(0) = \boldsymbol{u}_0$$

where γ is the diffusivity coefficient. This model can be considered in the class of general reaction-diffusion models of the kind: $\dot{\boldsymbol{u}}(t) = -\gamma L\boldsymbol{u}(t) + f(\boldsymbol{u}(t))$. A well-known model of this type is the Fisher-Kolmogorov-Petrovsky-Piskunov one [61, 62]. We propose to consider here the model in which $\gamma = 1$, and $0 \leq \boldsymbol{u}_0(i) < 1$. Also, because the graphs considered here are never the trivial one (edgeless graph), we always have that $\lambda_1 > 0$, so that by setting $\chi = 0$ we always guarantee the condition that $0 = \chi < \lambda_1$.

Then, we will consider that that a fraction of the concentration increased at the vertex i is removed from the node. Because $\boldsymbol{u}_0(i) < 1$ we consider that the fraction to be removed is equal to $\boldsymbol{u}_t(i)$ multiplied by the amount in which the concentration has increased:

$$\dot{u}_i(t) = \sum_{(j,i)\in E} A_{ij}u_j(t) - u_i(t)\sum_{(j,i)\in E} A_{ij}u_j(t)$$

which obviously represents the logistic equation on the graph:

$$\dot{u}_i(t) = (1 - u_i(t))\sum_{(j,i)\in E} A_{ij}u_j(t).$$

Our first goal here is to find approximate solutions by means of tight bounds of this equation on graphs rewritten in the following way (see [63]):

$$\frac{\dot{u}_i(t)}{1 - u_i(t)} = \sum_{(j,i)\in E} A_{ij}\left(1 - e^{-\left(-\log\left(1-u_j(t)\right)\right)}\right),$$

which can be written as $\frac{d\boldsymbol{y}(t)}{dt} = \sum_{(j,i)\in E} A_{ij} f\left(y_j(t)\right)$, where $y_i(t) \coloneqq -\log\left(1 - u_j(t)\right) \in [0, \infty]$, $f(y) \coloneqq 1 - e^{-y}$. Our concrete proposal is to obtain an upper bound to a linearised version of this equation which represents a good approximate solution of the logistic reaction-diffusion model considered here.

Based on our preliminary explorations of the problem we propose the following:

Working Plan

1. Use a linearisation of the form: $\frac{d\hat{y}(t)}{dt} = A\text{diag}(\boldsymbol{1} - \boldsymbol{u}_0)\hat{\boldsymbol{y}}(t) + b(\boldsymbol{u}_0)$, where $\hat{\boldsymbol{u}}(t) = f(\hat{\boldsymbol{y}}(t))$ approximates $\boldsymbol{u}(t)$.
2. Obtain the exact solution of the linearised logistic NC reaction-diffusion model and analyse the initial conditions on which the solution can be simplified without removing its physical meaning.

3. Analyse numerically how good the approximation obtained is to the exact solution of the model for different types of graphs/networks, studying the influence of several factors like degree heterogeneity, degree assortativity, existence of communities, etc.
4. Considering analytically the matrix functions emerging from the solution of the linearised problem under certain initial conditions. For instance, some of the solutions are related to matrix functions known as ψ-matrix functions, which are particular cases of the two-values Mittag-Leffler functions of a matrix M of the type: $E_{1,2}(M) = \frac{e^M - I}{M}$.
5. Compare the NC logistic model with conservative models of diffusion for the propagation of information on graphs/networks, by considering different types of topologies, in order to determine whether the NC diffusion displays advantages in terms of the speed of propagation in relation to conservative processes.

3.2. Spatial nonlocality in NC diffusion on graphs/networks

Participants: Ernesto Estrada (IFISC), PhD candidate

In this section of the project we will start by defining two new nonlocal operators on graphs. Let us first define the d-path degree of a vertex v as $k_{d,v} := \#\{w \in V : d(v,w) = d\}$, where $d(v,w)$ is the shortest path distance between the two vertices in G. Then, the d-path adjacency operator on the graph is defined as:

$$(\mathcal{A}_d f)(v) := \sum_{w \in V:\, d(v,w)=d} f(w).$$

In a similar way we extend the Lerman-Ghosh Laplacian operator to the d-path one:

$$(\mathcal{L}_{d,\chi} f)(v) = \sum_{w \in V:\, d(v,w)=d} \left(\frac{\chi}{k_{d,v}} f(v) - f(w) \right).$$

Let us now consider the following transformations of these operators. Let $diam = \max_{v,w \in V} d(v,w)$ be the diameter of the graph. Then,

$$\tilde{\mathcal{L}}_{\chi,\zeta} := \sum_{d=1}^{diam} e^{-\zeta d} \mathcal{L}_{d,\chi} \quad \text{and } \tilde{\mathcal{L}}_{\chi,s} := \sum_{d=1}^{diam} d^{-s} \mathcal{L}_{d,\chi},$$

are the Laplace- and Mellin-transformed d-path Lerman-Ghosh Laplacian operators with $\zeta > 0$ and $s > 0$, respectively. Notice that when $\chi = 0$ these operators are transformed into the Laplace- and Mellin-transformed d-path adjacency operators of the graph.

Working Plan

1. Investigate the general properties of the operators $\mathcal{A}_d$, $\mathcal{A}_{d,\{\zeta,s\}}$, $\mathcal{L}_{d,\chi}$, and $\tilde{\mathcal{L}}_{\chi,\{\zeta,s\}}$ on the basis of their boundedness and self-adjointness. In the case of the corresponding matrices we will focus on the analysis of their eigenvalues, particularly of the spectral radius of A_d, $\tilde{A}_{\{\zeta,s\}}$ and on the algebraic connectivity (second smallest eigenvalue) of $L_{d,\chi}$, and $\tilde{L}_{\chi,\{\zeta,s\}}$, for which we are interested in finding bounds based on simple graphs properties, such as the number of vertices, edges, maximum and minimum degree, etc.
2. Generalise the NC diffusion model by considering the spatially nonlocal Lerman-Ghosh Laplacians: $\dot{\boldsymbol{u}}(t) = -\tilde{L}_{\chi,\zeta}\, \boldsymbol{u}(t)$ and $\dot{\boldsymbol{u}}(t) = -\tilde{L}_{\chi,s}\, \boldsymbol{u}(t)$, proving their convergence in connected graphs, and the role played by $\mu_2(\tilde{L}_{\chi,\{\zeta,s\}}) = \min_{\mu_j \neq 0} \mu_j(\tilde{L}_{\chi,\{\zeta,s\}})$ in determining the rate of convergence of these processes.

3. Study computationally the main characteristic features of the spatially nonlocal NC diffusion models on an infinite linear chain to determine analytically whether there are conditions in which the process become super-diffusive, e.g., which transform (Mellin or Laplace) and which range on parameters on the corresponding transform.
4. Generalise the logistic NC diffusive model to consider spatial nonlocality via: $\dot{\boldsymbol{u}}(t) = \big(1-\boldsymbol{u}(t)\big)\tilde{A}_{\{\zeta,s\}}\boldsymbol{u}(t)$. Study the conditions needed to transform the model into linearised approximations of the form: $\frac{d\widehat{\boldsymbol{y}}(t)}{dt} = \tilde{A}_{\{\zeta,s\}}\mathrm{diag}(\mathbf{1}-\boldsymbol{u}_0)\widehat{\boldsymbol{y}}(t)+b(\boldsymbol{u}_0)$, where $\widehat{\boldsymbol{u}}(t) = f\big(\widehat{\boldsymbol{y}}(t)\big)$ approximates $\boldsymbol{u}(t)$. Then, analyse computationally the rate of convergence of this model to the steady state and compare it with the one without nonlocal spatial effects.
5. Study the NC diffusion models with spatial nonlocality on real-world networks, in particular to analyse diffusive processes in neuronal networks of different species, e.g., *C. elegans*, *D. melanogaster*, mouse and human, as well as to consider traffic in urban street networks at rush hours.

3.3. Temporal nonlocality in NC diffusion on graphs/networks

Participants: Ernesto Estrada (IFISC), PhD candidate

In this section of the project we will start by analysing a temporal nonlocal NC diffusion model with the Lerman-Ghosh Laplacian:

$$D_t^{\alpha}\boldsymbol{u}(t) = -L_{\chi}\boldsymbol{u}(t), \qquad \boldsymbol{u}(0) = \boldsymbol{u}_0,$$

where $D_t^{\alpha}\boldsymbol{u}(t)$ is the Caputo fractional derivative previously defined. The solution of this equation is given in terms of the Mittag-Leffler matrix functions $-E_{\alpha}\big(L_{\chi}\big)$:

$$\boldsymbol{u}(t) = -E_{\alpha}\big(L_{\chi}\big)\,\boldsymbol{u}_0,$$

We then proceed to define and study temporally nonlocal logistic NC diffusion models of the type:

$$D_t^{\alpha}\boldsymbol{u}(t) = \big(1-\boldsymbol{u}(t)\big)A\boldsymbol{u}(t), \qquad \boldsymbol{u}(0) = \boldsymbol{u}_0.$$

Working Plan

1. Proving the convergence conditions of the model $D_t^{\alpha}\boldsymbol{u}(t) = -L_{\chi}\boldsymbol{u}(t)$ and compare them with the ones obtained for the standard NC model, particularly by considering the influence of the fractional parameter α on the rate of convergence.
2. Prove whether the fractional NC diffusive model can give rise to sub-diffusive behaviour on graphs using an infinite linear chain. Show the conditions, in terms of the parameter α, which change the behaviour of the system from normally diffucive to sub-diffusive.
3. Investigate the spectral properties of the Mittag-Leffler matrix functions of the Lerman-Ghosh Laplacian $E_{\alpha}\big(L_{\chi}\big)$. Then, obtaine analogous of **Lemma 1** in which we find $\lim_{t\to\infty}\boldsymbol{u}(t)$ as a function of χ and the spectra of $E_{\alpha}\big(L_{\chi}\big)$.
4. Study the conditions needed to transform the logistic fractional NC diffusion model into linearised approximations of the form: $D_t^{\alpha}\boldsymbol{u}(t) = A\mathrm{diag}(\mathbf{1}-\boldsymbol{u}_0)\widehat{\boldsymbol{y}}(t)+b(\boldsymbol{u}_0)$, where $\widehat{\boldsymbol{u}}(t) = f\big(\widehat{\boldsymbol{y}}(t)\big)$ approximates $\boldsymbol{u}(t)$. Then, analyse computationally the rate of convergence of this model to the steady state and compare it with the one without nonlocal spatial effects.

5. Study the NC diffusion models with temporal nonlocality on real-world networks, in particular to analyse diffusive processes in neuronal networks of different species, e.g., *C. elegans*, *D. melanogaster*, mouse and human, as well as to consider traffic in urban street networks at rush hours.

3.4. Time-and-space nonlocal NC diffusion on graphs/networks

Participants: Ernesto Estrada (IFISC), PhD candidate

The main goal of this section of the project is to generalise NC diffusion to include simultaneously time and space nonlocality via fractional time derivatives and transformed d-path Lerman-Ghosh Laplacians, respectively:

$$D_t^{\alpha}\boldsymbol{u}(t) = -\tilde{L}_{\chi,\{\zeta,s\}}\,\boldsymbol{u}(t), \qquad \boldsymbol{u}(0) = \boldsymbol{u}_0,$$

whose solution is of the form:

$$\boldsymbol{u}(t) = -E_{\alpha}\left(\tilde{L}_{\chi,\{\zeta,s\}}\right)\boldsymbol{u}_0,$$

for the Laplace (ζ) and Mellin (s) transformations, respectively.

We will also study here a spatial and temporally nonlocal logistic NC diffusion models of the type:

$$D_t^{\alpha}\boldsymbol{u}(t) = \left(1 - \boldsymbol{u}(t)\right)A_{\{\zeta,s\}}\boldsymbol{u}(t), \qquad \boldsymbol{u}(0) = \boldsymbol{u}_0,$$

where $A_{\{\zeta,s\}}$ are the Laplace and Mellin transformed d-path adjacency matrices of the graph, respectively.

Working Plan

1. Proving the convergence conditions of the model $D_t^{\alpha}\boldsymbol{u}(t) = -\tilde{L}_{\chi,\{\zeta,s\}}\,\boldsymbol{u}(t)$, and find the combined conditions which transform the process from normal diffusion to sub- and super-diffusion.
2. Study the conditions needed to transform the time-and-space nonlocal logistic NC diffusion model into linearised approximations of the form: $D_t^{\alpha}\boldsymbol{u}(t) = A_{\{\zeta,s\}}\mathrm{diag}(\boldsymbol{1} - \boldsymbol{u}_0)\hat{\boldsymbol{y}}(t) + b(\boldsymbol{u}_0)$, where $\hat{\boldsymbol{u}}(t) = f\left(\hat{\boldsymbol{y}}(t)\right)$ approximates $\boldsymbol{u}(t)$. Then, analyse computationally the rate of convergence of this model to the steady state and compare it with the one without nonlocal spatial effects.
3. Study the NC diffusion models with temporal and spatial nonlocality on real-world networks, in particular to analyse diffusive processes in neuronal networks of different species, e.g., *C. elegans*, *D. melanogaster*, mouse and human, as well as to consider traffic in urban street networks at rush hours.

3.5. Geometry of generalised NC diffusions on graphs/networks

Participants: Ernesto Estrada (IFISC), PhD candidate

In the standard NC diffusion model with the Lerman-Ghosh Laplacian the solution is given in terms of the semigroup $e^{-tL_{\chi}}$. Thus, at a given time the potential at a given pair of vertices is:

$u_t(v) = \sum_j \left(e^{-tL_\chi}\right)_{vj} u_0(j)$ and $u_t(w) = \sum_j \left(e^{-tL_\chi}\right)_{wj} u_0(j)$. Then, if we consider the flow between the two vertices when the initial potential was at vertex v, we have:

$$\mathcal{F}_{vw|u_0(j)=\delta_{jv}}(t) = u_{v|u_0(j)=\delta_{jv}}(t) - u_{w|u_0(j)=\delta_{jv}}(t),$$

and the other way around,

$$\mathcal{F}_{wv|u_0(j)=\delta_{jw}}(t) = u_{w|u_0(j)=\delta_{jw}}(t) - u_{v|u_0(j)=\delta_{jw}}(t).$$

Consequently, the "traffic" in both directions between the pairs of vertices v and w is given by:

$$\mathcal{D}_{vw}\left(L_\chi, t\right) \coloneqq \mathcal{F}_{vw|u_0(j)=\delta_{jv}}(t) + \mathcal{F}_{wv|u_0(j)=\delta_{jw}}(t) = \left(e^{-tL_\chi}\right)_{vv} + \left(e^{-tL_\chi}\right)_{ww} - 2\left(e^{-tL_\chi}\right)_{vw}.$$

Proposition 2. $\mathcal{D}_{vw}(t)$ is a square circum-Euclidean distance between the vertices v and w of the graph.

Also, because $e^{-tL_\chi} = e^{-t\chi}e^{tA}$ we have that.

$$\mathcal{D}_{vw}\left(L_\chi, t\right) = e^{-t\chi}[(e^{tA})_{vv} + (e^{tA})_{ww} - 2(e^{tA})_{vw}],$$

where the term in the brackets is the communicability distance.

Working Plan

1. Define and study the properties of the circum-Euclidean distance $\mathcal{D}_{vw}\left(\tilde{L}_{\chi,\{\zeta,s\}}, t\right) = e^{-t\chi}\left[\left(e^{tA_{\{\zeta,s\}}}\right)_{vv} + \left(e^{tA_{\{\zeta,s\}}}\right)_{ww} - 2\left(e^{tA_{\{\zeta,s\}}}\right)_{vw}\right]$ emerging from the solution of the spetially nonlocal NC diffusion model.
2. Study the circum-Euclidean embedding of the graphs induced by $\mathcal{D}_{vw}\left(\tilde{L}_{\chi,\{\zeta,s\}}, t\right)$ by defining and studying the radius of the hypersphere where the embedding takes place, the angles between the position vectors of the vertices on the surface of the hypersphere and other geometric parameters.
3. Study the geometrization of graphs based on $\mathcal{D}_{vw}\left(\tilde{L}_{\chi,\{\zeta,s\}}, t\right)$ and study the trajectories of diffusive particles between origin-destination pairs based on the corresponding shortest paths. Compare them with the ones produced by NC diffusion without space nonlocality as well as with conservative diffusion.
4. Define and study the properties of distances of the form: $\mathcal{E}_{vw}(A, t) \coloneqq \left(E_\alpha(A)\right)_{vv} + \left(E_\alpha(A)\right)_{ww} - 2\left(E_\alpha(A)\right)_{vw}$, which emerge in the solution of temporal nonlocal NC diffusion on graphs. Analyse the conditions determining that the embedding induced by these distances is circum-Euclidean and study properties of it, such as angles between position vectors, radius of hyperspheres, etc.
5. Define and study the properties of distances of the form: $\mathcal{E}_{vw}\left(A_{\{\zeta,s\}}, t\right) \coloneqq \left(E_\alpha\left(A_{\{\zeta,s\}}\right)\right)_{vv} + \left(E_\alpha\left(A_{\{\zeta,s\}}\right)\right)_{ww} - 2\left(E_\alpha\left(A_{\{\zeta,s\}}\right)\right)_{vw}$, which emerge in the solution of time-and-space nonlocal NC diffusion on graphs. Analyse the conditions determining that the embedding induced by these distances is circum-Euclidean and study properties of it, such as angles between position vectors, radius of hyperspheres, etc.
6. Study the geometrization of graphs based on $\mathcal{E}_{vw}\left(A_{\{\zeta,s\}}, t\right)$ and study the trajectories of diffusive particles between origin-destination pairs based on the corresponding shortest paths. Compare them with the ones produced by NC diffusion without space, and time nonlocality as well as with conservative diffusion.
7. Study the geometries induced by time-and-space nonlocal NC diffusion models on real-world networks, in particular to analyse diffusive processes in neuronal networks of

different species, e.g., *C. elegans*, *D. melanogaster*, mouse and human, as well as to consider traffic in urban street networks at rush hours.

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IMPACTO ESPERADO DE LOS RESULTADOS - *EXPECTED RESULTS IMPACT*

This project has two major areas of scientific impact. The first is logically in the mathematical study of graphs and networks in general and in the study of algebraic theory of graphs. The second is in the areas of applications of graphs and networks to the study of complex systems. The Laplacian operator of the graph is one of the most studied algebraic objects in graph theory. Its importance is that it contains great structural information about the graph. For example, the algebraic properties of the Laplacian are related to the number of spanning trees in the graph, to its connectivity, to its isoperimetric and expansion properties, to the random walker model in the graph, to the speed of convergence of diffusive dynamics, to the synchronizability of a network of oscillators, among others. In the study of complex networks, the Laplacian plays a vital role in the understanding of diffusion, synchronization, consensus protocols in autonomous systems, controllability of networks, pattern formation, signal processing, detection of communities and the analysis of electrical networks, among many others. It is worth noting that diffusion and synchronization are processes that occur in molecular, neuronal and cellular networks, in social systems, in ecological systems, between financial and infrastructure entities.

The introduction of the hubs-repelling/attracting Laplacian operators proposed in this project will therefore have a direct impact on the understanding of the structural properties of graphs and how they affect the dynamics that occur in them. There is experimental evidence that shows the possible existence of diffusive processes with hubs-repulsion in real systems. An example is the diffusion processes in the brain, where the energy cost increases with the connectivity of the node, so diffusive particles would avoid the nodes of greater degree. Another example is the propagation of flight delays in air transport networks, where the most connected airports have a better capacity to absorb such delays, which would accumulate mostly in smaller airports. With the mathematical tools to be developed in this project, these scenarios and many others, can be studied both analytically and through computer simulations for their better understanding.

To reach the widest possible audience during the project, we will disseminate our results in both specialized journals and high-impact interdisciplinary journals. All this information will be available in the form of open access material. We will promote the project by participating in specialized conferences and workshops on the subject, as well as in the main conferences of applied mathematics and complex networks.

All previous dissemination processes will help achieve the expected impact of the project by providing long-term links to users in Spain and Europe. Fundamentally, in this project we will have a wide network of external collaborators who will help convince the international scientific community of the importance and need for a wide use of our theoretical tools.

Specifically, the dissemination of the results of this project includes several aspects:

- Publication in regular journals and assistance to scientific conferences;
- Collaborations with other groups as mentioned in the memory;
- Disseminating our results through the media;
- Dissemination on personal web page.

1. CAPACIDAD FORMATIVA *TRAINING CAPACITY*

1.1. Programa de formación previsto en el contexto del proyecto solicitado. *Training program planned in the context of the requested project*

1.2. Tesis realizadas o en curso en el ámbito del equipo de investigación (últimos 10 años). *Theses completed or in progress within the scope of the research team (last 10 years).*

Period	Name	Thesis title

2012-2015	Eusebio Vargas Estrada	Leader-follower consensus under peer-pressure in complex networks
2015-2018	Matthew Sheerin	Random rectangular networks: theory and applications
2016-2019	Ehsan Mejeed Hameed	Mathematical analysis of d-path Laplacian operators in simple graphs.
2016-2019	Grant Russell Silver	Matrix function analysis of graphs and networks.
2017-2022	Alhanouf A. Alhomaidhi	Spectral folding and related matrix functions for graph/network analysis

1.2. Theses in progress in the group

Period	Name	Thesis title
2021-2024	Fernando Diaz Diaz	Estudio de redes con signos y sus aplicaciones.
2021-2024	Manuel Miranda	Dinámicas difusivas y advectivas en grafos y redes.

6.3 Professional development of Doctors graduated in our group

The first graduated Doctor from our group was Dr. Santiago Vilar who after having positions as researcher at National Institute of Diabetes and Digestive and Kidney Diseases at the National Institutes of Health (USA) and at the Department of Biomedical Informatics at Columbia University (New York, USA) is currently a Computational Chemist at Polaris, in Durham, USA. The second graduated Doctor was Dr. Frack Kalala-Mutombo, who is currently Academic Manager at the African Institute of Mathematical Sciences (AIMS) in Senegal. The third one, Dr. Eusebio Vargas-Estrada, after graduation from our group held a Research Assistant position at the University of Konstanz, Germany, with Prof. Ulrik Brandes, and as Professor at the Pontificia Universidad Católica de Valparaiso in Chile is now Professor at the prestigious Tecnológico de Monterrey in Mexico. After graduation Dr. Matthew Sheerin took a position as Software Engineer at Metaswitch Networks in Edinburgh, U.K. Dr. Grant Silver is nowadays Senior Project Analyst at Quick Release (Automotive) Ltd in Greater Glasgow Area, U. K. Dr. Ehsan Majeed Hameed returned to Iraq where he holds a position as Professor at the University of Thi-Qar. After her graduation Dr. Alhanouf Ali Alhomaidhi (female) is currently Assistant Professor at King Saud University in Riyadh, Saudi Arabia.

6.4 Scientific and formative capacity of the team and institution