NUMERICAL APPROXIMATION OF NONHOMOGENEOUS BOUNDARY CONDITIONS ON NETWORKS FOR A HYPERBOLIC SYSTEM OF CHEMOTAXIS MODELING THE PHYSARUM DYNAMICS

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ABSTRACT. Many studies have shown that Physarum polycephalum slime mold is able to find the shortest path in a maze. In this paper we study this behavior in a network, using a hyperbolic model of chemotaxis. Suitable transmission and boundary conditions at each node are considered to mimic the behavior of such an organism in the feeding process. Several numerical tests are presented for special network geometries to show the qualitative agreement between our model and the observed behavior of the mold.

1. Introduction. In recent years, the behavior of Physarum polycephalum, a “many-headed” slime mold with multiple nuclei, has been studied in depth and considered as a model organism representing amoeboid movement and cell motility. We underline that here we are not interested in describing the biological mechanism of growth of bacteria, but only their movement under chemical stimuli, then the growth mechanism will be neglected. The body of the plasmodium, representing the main vegetative phase of Physarum polycephalum, contains a network of tubes (pseudopodia), by means of which nutrients and chemical signals circulate throughout the organism [21]; the flow in the tube is bidirectional, as it can be observed to switch back and forth. The movement is characterized by cytoplasmic streaming, driven by rhythmic contractions of organism, that sustains and reorganizes tubes: a larger flow leads to a wider tube.

An example of the behavior of starved plasmodium searching for food has been shown in an experiment performed by Nakagaki, Yamada, and Tóth in [21]. First, they built a maze on an agar surface. Therefore, they put over the agar surface some parts of the plasmodium, which started to spread...
and coalesced to form a single organism that filled the maze. After that, they placed agar blocks containing oatmeal at the exits and, after some hours, they observed the dead ends of the plasmodium shrank (the tubes with a smaller flux ended to disappear) and the colony, after exploring all possible connections, produced the formation of a single thick pseudopodium spanning the minimum distance between the food sources. See for instance some popular videos freely available on the web, as for instance this one [29]. Then, to summarize, the main features in the evolution of the slime mold system are the following two steps: dead end cutting, and the selection of the solution path among the competitive paths. This behavior can be applied to both path-finding in a maze and path selection in a transport network. The ability of solving this kind of problems of an unicellular organism has been deeply investigated using various mathematical models. The hydrodynamic properties of the transportation of flux by the tubes of plasmodium and the mechanisms under the rhythmic oscillation of Physarum were investigated in [24], and biologically inspired models for adaptive network construction were developed [26] and [28].

A mathematical model based on ordinary differential equations to describe the adaptation process of the tube network peculiar in the dynamics of Physarum was introduced in [25]. The ODE model is based on a regulation mechanism, which balances the system between the thickness of a tube and the flux through it. In that paper, it was shown numerically that, in the asymptotic steady state of the model, the solution converges to the minimum-length solution between a source and a sink on any input graph. The theoretical analysis of such ODE model was carried out in successive works such as [18, 19, 1]. In particular, in [18] there was the proof of convergence for two parallel links, while the convergence of this model for any network to the shortest path connecting the source and the sink was analytically proved in [1].

Another modeling approach is represented by partial differential equations. In fact, the movement of individuals under the effect of a chemical stimulus of chemoattractant has been widely studied in mathematics in the last two decades, see [15, 20, 23], and various models involving partial differential equations have been proposed. This process is known as chemotaxis: the organism will move with higher probability towards food sources and it will produce an attractive chemical substance, usually a chemokine. The basic unknowns in these chemotactic models are the density of individuals and the concentrations of some chemical attractants. One of the most considered models of this type is the Patlak-Keller-Segel system [16], where the evolution of the density of cells is described by a parabolic equation, and the concentration of a chemoattractant is generally given by a parabolic or elliptic equation, depending on the different regimes to be described and on authors’ choices. The analytical study of the KS model on networks was presented in the recent paper [5], where the existence of a time global and spatially continuous solution for both the doubly parabolic and the
parabolic-elliptic systems was proved. By contrast, models based on hyperbolic/kinetic equations for the evolution of the density of individuals, are characterized by a finite speed of propagation [8, 23, 7, 6, 13].

In this paper, we deal with a hyperbolic-parabolic model, originally considered in [27], and later reconsidered in [12], which arises as a simple model for chemotaxis on a line:

\[
\begin{aligned}
& u_t + v_x = 0, \\
& v_t + \lambda^2 u_x = \chi \phi_x u - v, \\
& \phi_t - D \phi_{xx} = au - b\phi.
\end{aligned}
\] (1)

The function \( u \) is the density of individuals in the considered medium, \( v \) is their averaged flux and \( \phi \) denotes the density of chemoattractant. The individuals move at a constant speed \( \lambda \geq 0 \), changing their direction along the axis during the time. The positive constant \( D \) is the diffusion coefficient of the chemoattractant; the positive coefficients \( a \) and \( b \), are respectively its production and degradation rates, and \( \chi \) is the chemotactic sensitivity. Let us underline that the flux \( v \) in model (1) corresponds to \( v = -\lambda^2 u_x + \chi \phi_x u \) for the parabolic KS system. This system was analytically studied on the whole line and on bounded intervals in [13], while an effective numerical approximation, the Asymptotic High Order (AHO) scheme, was proposed in [22], see also [10, 11]. The AHO scheme was introduced in order to balance correctly the source term with the differential part and avoid an incorrect approximation of the density flux at equilibrium. These schemes are based on standard finite differences methods, modified by a suitable treatment of the source terms, and they take into account, using a Taylor expansion of the solution, the behavior of the solutions near non constant stationary states.

Model (1) can also be considered on a network, where solutions on each arc are coupled through transmission conditions ensuring the total continuity of the fluxes at each node, while the densities can have jumps. The first analytical study of this model on a network was given in [14], where a global existence result of solution for suitably small initial data was established. Note that transmission conditions in [14] are imposed in a different way respect to the present paper, but they may coincide for particular choices of the transmission coefficients, such as for conditions (43) in Section 4. Concerning the numerical approximation, in [4] we extended the AHO scheme of [22] to the case of networks. In this case, a particular attention was paid to the proper setting of conditions at internal and external nodes in order to guarantee the conservation of the total mass.

In the present paper, starting from the work in [4] and inspired by the study on a doubly parabolic chemotaxis system presented in [3, 5], where the one-dimensional KS model was extended to networks, we present a numerical study of amoeboid movements, using the hyperbolic chemotaxis model (1) on networks connecting two or more exits. The main difference with works on chemotaxis based on parabolic equations is not only the hyperbolicity of
the equations describing the cell movement, but the transmission conditions, which in our case, unlike what was assumed in [3, 5], are designed to allow for discontinuous densities at each node. Actually, this condition is believed to be more appropriate when considering a flow of individuals on a network, see for instance [9] and references therein and also the recent discussion in [2]. Then, to summarize, the model (1) has the following peculiar features:

- discontinuous conditions on densities at the junctions of the network;
- finite speed of propagation for cells.

Regarding the numerical approximation of (1), we refer to [4], where the numerical approximation of the hyperbolic part of the system is based on the AHO scheme, while the parabolic part is approximated with the Crank-Nicolson scheme. However, differently from [4], we need to deal with more general Neumann boundary conditions. In fact, the main aspect of this paper is the introduction of more general boundary conditions to take into account non homogeneous boundary conditions both for the density and the chemoattractant. From the modeling point of view this is motivated by the necessity of including the inflow of cells and the food providing at the network exits, therefore we assume inflow boundary conditions at external nodes both for the density of cells and the chemoattractant.

The mentioned scheme, complemented with general Neumann boundary conditions, will be used to obtain numerical solutions for networks with special geometries, motivated by experimental observations. Let us notice that the properties of dead-end cutting and shortest path selection in our model are represented by different mass distribution on the edges of the assigned network described as an oriented graph. We also underline that in subsection 4.2.3 we considered the case of a network with more than two exits. This is the first time that this case is considered with a PDE chemotaxis model. Furthermore, to our knowledge, the feeding process in such cases have not been fully described yet with ODE models.

The paper is organized as follows. In Section 2 we describe the main setting of problem (1). Section 3 is devoted to the description of the numerical approximation of the problem based on the AHO scheme of second order with a suitable discretization of the transmission and boundary conditions for the case of non-null Neumann boundary conditions. In particular, a strong emphasis will be given to formulate the correct boundary conditions for the AHO schemes for the inflow and outflow cases. Finally, in Section 4, we report some numerical tests for the distribution of densities within networks of different topologies, having in mind the laboratory experiments made with Physarum, in order to test the correspondence between our simulations and the real behavior of such an organism. In this framework, a comparison between the results obtained with the two models, the one in [3] and the present one, is also provided, showing substantially the same asymptotic behavior of the solutions, even if the transmission conditions at
each node are not the same, and so the transitory profiles.

2. Analytical framework. First, let us represent a network as a connected graph. We define a connected graph $G = (N, A)$ as formed by two finite sets, a set of $P$ nodes (or vertices) $N$ and a set of $N$ arcs (or edges) $A$, such that an arc connects a pair of nodes. Since arcs are bidirectional the graph is non-oriented, but we need to fix an artificial orientation in order to fix a sign to the velocities. The network is therefore composed of “oriented” arcs and there are two different types of intervals at a node $p \in N$: incoming ones – the set of these intervals is denoted by $I_p$ – and outgoing ones – whose set is denoted by $O_p$. For example, on the network depicted in Figure 1, $1 \in I_1$ and $2, 3 \in O_1$. We will also denote in the following by $I_{out}$ and $O_{out}$ the set of the arcs incoming or outgoing from the outer boundaries. The $N$ arcs of the network are parametrized as intervals $[0, L_i]$, $i = 1, \ldots, N$, and for an incoming arc, $L_i$ is the abscissa of the node, whereas it is 0 for an outgoing arc.

We consider system (1) on each arc and rewrite it in diagonal variables for its hyperbolic part by setting

$$u^\pm = \frac{1}{2} \left( u \pm \frac{v}{\lambda} \right).$$

Here $u^+$ and $u^-$ are the Riemann invariants of the system and $u^+$ (resp. $u^-$) denotes the density of cells following the orientation of the arc (resp. the density of cells going in the opposite direction). This transformation is inverted by $u = u^+ + u^-$ and $v = \lambda(u^+ - u^-)$, and yields:

$$\begin{align*}
&u^+_i + \lambda u^+_x = \frac{1}{2\lambda} \left( (\chi \phi_x - \lambda)u^+ + (\chi \phi_x + \lambda)u^- \right), \\
&u^-_i - \lambda u^-_x = -\frac{1}{2\lambda} \left( (\chi \phi_x - \lambda)u^+ + (\chi \phi_x + \lambda)u^- \right), \\
&\phi_t - D\phi_{xx} = a(u^+ + u^-) - b\phi.
\end{align*}$$

We complement this system by initial conditions at $t = 0$ on each arc

$$u^+_i(x, 0) = u^+_0(x), \quad u^-(x, 0) = u^-_0(x), \quad \phi(x, 0) = \phi_0(x), \quad \text{for } x \in [0, L],$$

with $u^+_0, \quad u^-_0, \quad \phi_0$ some $C^3$ functions.

Up to now, we omitted the indexes related to the arc number since no confusion was possible. From now on, however, we need to distinguish the quantities on different arcs and we denote by $u^+_i, \quad u^-_i, \quad v_i, \quad \phi_i$ etc., the values of the corresponding variables on the $i$-th arc.

On the outer boundaries, we consider the more general boundary conditions:

$$\begin{align*}
u^+_i(0, t) = g_i(t, u^-_i(0, t)), \quad \text{if } i \in O_{out}, \\
u^-_i(L_i, t) = g_i(t, u^+_i(L_i, t)), \quad \text{if } i \in I_{out},
\end{align*}$$

(4)
for some nonlinear smooth function \( g_i(t, u) \), corresponding to general boundary conditions on the flux function \( v \):

\[
\begin{align*}
  v_i(0, t) &= w(0, t), \quad \text{if } i \in O_{\text{out}}, \\
  v_i(L_i, t) &= z(L_i, t), \quad \text{if } i \in I_{\text{out}},
\end{align*}
\]

with \( w, z \) two functions eventually depending on \( u(\cdot, t) \). We can also assume more general conditions for the flux of chemoattractant at the outer boundaries, also including the null Neumann condition. Indeed, considering the normal derivative of chemoattractant at an outer node, we can assume the following general condition:

\[
\partial_n \phi_i(\cdot, t) + \beta \phi_i(\cdot, t) = \bar{\phi}_i(t),
\]

with parameter \( \beta \geq 0 \) and \( \bar{\phi}_i \) a given non-negative function varying in time that reproduces the inflow/outflow of nutrient substances. In particular, if \( \bar{\phi}_i > \beta \phi_i(\cdot, t) \) this leads to a higher concentration of the chemoattractant at the outer nodes; if, on the contrary, \( \bar{\phi}_i < \beta \phi_i(\cdot, t) \), this represents the decrease of chemoattractant at the outer boundaries.

Note that in the sequel we will also consider the subcase of \( \beta = 0 \) and \( \bar{\phi} \) constant in time, also including constantly null boundary conditions.

2.1. Transmission conditions. We briefly recall transmission conditions imposed at inner nodes in our previous work [4]. We underline that transmission conditions on \( u \) ensure the continuity of fluxes at each node, but not the continuity of the densities; however, the continuity of the fluxes is enough since it implies that we cannot loose nor gain any cells during the passage through a node. In the case of non-vanishing Neumann conditions at the outer boundaries, implemented for the first time in this paper, the conservation of the global mass of the system obviously does not hold. If we consider the case treated in the numerical tests in Section 4, we have two arcs connected to the outer boundaries (a source and a sink), say arcs \( l \) and \( m \). In such a case we have that the derivative in time of the total mass \( \mu \) is given by:

\[
\mu'(t) = v_l(0, t) - v_m(L_m, t), \quad \text{for all } t > 0.
\]

As in [4], we do not impose the continuity of the density of chemoattractant \( \phi \), but only the continuity of the flux at node \( p \in \mathcal{N} \). Therefore, we use the Kedem-Katchalsky permeability conditions [17] at each node:

\[
D_i \partial_n \phi_i = \sum_{j \in I_p \cup O_p} \kappa_{i,j} (\phi_j - \phi_i), \quad i \in I_p \cup O_p,
\]

for some positive coefficients \( \kappa_{i,j} \), and, under the condition \( \kappa_{i,j} = \kappa_{j,i}, \quad i, j = 1, \ldots, N \) the conservation of the fluxes at node \( p \) holds, that is to say:

\[
\sum_{i \in I_p \cup O_p} D_i \partial_n \phi_i = 0.
\]
Note that setting $\kappa_{i,i} = 0$, $i = 1, \ldots, N$, does not change condition (8), and the positivity of the transmission coefficients $\kappa_{i,j}$ guarantees the energy dissipation for the equation for $\phi$ in (1), when the term in $u$ is absent.

Now, at node $p \in \mathcal{N}$ we have to give values to the components such that the corresponding characteristics are going out of the node. Therefore, we consider the following transmission conditions at node:

\[
\begin{align*}
&u_i^- (L_i, t) = \sum_{j \in I_p} \xi_{i,j} u_j^+ (L_j, t) + \sum_{j \in O_p} \xi_{i,j} u_j^- (0, t), \text{ if } i \in I_p, \\
&u_i^+ (0, t) = \sum_{j \in I_p} \xi_{i,j} u_j^+ (L_j, t) + \sum_{j \in O_p} \xi_{i,j} u_j^- (0, t), \text{ if } i \in O_p,
\end{align*}
\]

where the constant $\xi_{i,j} \in [0, 1]$ are the transmission coefficients: they represent the probability that a cell at a node decides to move from the $i$-th to the $j$-th arc of the network, also including the turnabout on the same arc. These transmission conditions do not guarantee the continuity of the densities at node; however, we are interested in having the continuity of the fluxes at the node, meaning that we cannot loose nor gain any cells during the passage through a node. This is obtained using a condition mixing the transmission coefficients $\xi_{i,j}$ and the velocities of the arcs connected at node $p$. We also recall that, since the transmission conditions at a node give the coupling between the densities on the arcs, in order to have the flux conservation, it is enough to impose the following condition at each node $p \in \mathcal{N}$, see [4] for the details:

\[
\sum_{i \in I_p \cup O_p} \lambda_i \xi_{i,j} = \lambda_j, \text{ } j \in I_p \cup O_p, \tag{10}
\]

and at each node $p$, we have:

\[
\sum_{j \in I_p \cup O_p} \xi_{i,j} = 1 \text{ for all } i \in I_p \cup O_p. \tag{11}
\]

3. A numerical approximation for system (1). Here we extend the numerical scheme introduced in [4] to the case of non-vanishing Neumann boundary conditions.

3.1. Approximation of the hyperbolic equations of the system in the case of a network. Let us consider a network as previously defined. Each arc $a_i \in \mathcal{A}$, $1 \leq i \leq N$, is parametrized as an interval $a_i = [0, L_i]$ and is discretized with a space step $h_i$ and discretization points $x^j_i$ for $j = 0, \ldots, M_i + 1$. We still denote by $k$ the time step, which is the same for all the arcs of the network. In this subsection, we denote by $w_{i,j}^{n}$ the discretization on the grid at time $t_n$ and at point $x^j_i$ of a function $w_i$, $i = 1, \ldots, N$ on the $i$-th arc for $j = 0, \ldots, M_i + 1$ and $n \geq 0$. Here we describe the discretization of system (1) on each arc, denoting by $f = \chi \phi_x u$ and omitting the parabolic
equation for $\phi$. We therefore consider the following system

$$\begin{aligned}
&u_t + v_x = 0, \\
v_t + \lambda^2 u_x = f - v,
\end{aligned} \quad (12)$$

and rewrite it in a diagonal form, using the usual change of variables (2),

$$\begin{align*}
&u_t - \lambda u_x = \frac{1}{2}(u^+ - u^-) - \frac{1}{2\lambda} f, \\
u_t + \lambda u_x = \frac{1}{2}(u^- - u^+) + \frac{1}{2\lambda} f.
\end{align*} \quad (13)$$

On each arc we consider the second order AHO scheme (the scheme is second order in the sense specified in the remark below) written in diagonal variables:

$$\begin{align*}
&u_{n+1,i}^{n+1,j} = \left(1 - \lambda \frac{h_i}{n_i} - \frac{k}{4}\right) u_{n,i}^{n,j} + \left(\frac{h_i \lambda}{n_i} - \frac{k}{4}\right) u_{n,j}^{n,j} + \frac{k}{4} (u_{n,j}^{n,j} + u_{n,j}^{n,j+1}) \\
&\quad - \frac{k}{4h_i} (f_{n,j}^{n,j+1} + f_{n,j}^{n,j}), \quad j = 0, \ldots, M_i, i = 1, \ldots, N, \quad (14) \\
&u_{n+1,i}^{n+1,j} = \left(1 - \lambda \frac{h_i}{n_i} - \frac{k}{4}\right) u_{n,i}^{n,j} + \left(\frac{h_i \lambda}{n_i} - \frac{k}{4}\right) u_{n,j}^{n,j-1} + \frac{k}{4} (u_{n,j}^{n,j} + u_{n,j}^{n,j-1}) \\
&\quad + \frac{k}{4h_i} (f_{n,j}^{n,j-1} + f_{n,j}^{n,j}), \quad j = 1, \ldots, M_i + 1, i = 1, \ldots, N. \quad (15)
\end{align*}$$

**Remark 1.** Note that we have a second–order AHO scheme on every stationary solutions, which is enough to balance the flux of the system at equilibrium, see [22] for more details. For simplicity here we only deal with second order schemes, but third order schemes could also be considered.

3.1.1. **Boundary conditions.** The boundary conditions needed on each arc are two boundary conditions at the endpoints linked to external nodes and two transmission conditions at the endpoints linked to internal nodes. Considering an arc in a network and its initial and end nodes, there are two possibilities for each node: either it is external, namely a node from the outer boundary linked to only one arc, or it is internal and it connects several arcs together. The boundary and transmission conditions will therefore depend on this feature. The no-flux boundary condition at outer nodes and the transmission conditions at inner nodes were already presented in a previous work, see [4].

Here we consider the more general case of non vanishing Neumann boundary conditions, which is finally the main goal of this section. Let us consider a general inflow condition at the nodes $p_1$ and $p_2$, with $w, z$ two functions eventually depending on $u$ and computed at the first or last endpoint of the arc, respectively:

$$v_l(0, t) = w(0, t), \ l \in O_{p_1} \quad (16)$$

$$v_m(L_m, t) = z(L_m, t), \ m \in I_{p_2}, \quad (17)$$

and we consider the exact discretization on the grid (thus keeping the AHO scheme of first order during the evolution and of second order on stationary
solution:

\[
\begin{align*}
\frac{v_{l}^{n+1,0}}{w^{n+1,0}}, & \quad l \in O_{p_{1}} \\
\frac{v_{m}^{n+1,M_{m}+1}}{z^{n+1,M_{m}+1}}, & \quad m \in I_{p_{2}}.
\end{align*}
\]

(18)

**Remark 2.** In particular, in the case of the networks considered in Section 4, in order that a certain amount of the organism enters into the network by the node \(p_{1}\), at the outer boundaries we have the inflow conditions:

\[
v_{l}(0, t) = \frac{2}{1 + u_{l}(0, t)} , \quad l \in O_{p_{1}}
\]

(19)

for an arc \(l\) exiting from the source node \(p_{1}\) and, analogously, for an arc \(m\) entering the sink node \(p_{2}\) we set:

\[
v_{m}(L_{m}, t) = \frac{-2}{1 + u_{m}(L_{m}, t)} , \quad m \in I_{p_{2}}.
\]

(20)

Since in the general case of non-null Neumann conditions the conservation of the total mass of the system does not hold, we need to compute the numerical approximation scheme at the outer boundaries in such a case, taking into account the relation (7). The discrete total mass is given by

\[
I_{n}^{n+1}_{\text{tot}} = \sum_{i=1}^{N} I_{n}^{n}_{i},
\]

where the mass corresponding to the arc \(i\) is defined as:

\[
I_{n}^{n}_{i} = h_{i} \left( \frac{u_{i}^{n,0}}{2} + \sum_{j=1}^{M_{i}} u_{i}^{n,j} + \frac{u_{i}^{n,M_{i}+1}}{2} \right)
\]

\[
= h_{i} \left( \frac{u_{i}^{n,0} + u_{i}^{n,0}}{2} + \sum_{j=1}^{M_{i}} (u_{i}^{n,j} + u_{i}^{n,j}) + \frac{u_{i}^{n,M_{i}+1} + u_{i}^{n,M_{i}+1}}{2} \right).
\]

Computing \(I_{n}^{n+1}_{\text{tot}} - I_{n}^{n}_{\text{tot}}\), we find:

\[
I_{n}^{n+1}_{\text{tot}} - I_{n}^{n}_{\text{tot}} = \sum_{i=1}^{N} h_{i} k \left( \frac{1}{k}(u_{i}^{n+1,0} - u_{i}^{n+1,0}) + \frac{1}{k}(u_{i}^{n+1,0} - u_{i}^{n+1,0}) + (\frac{2\lambda_{i}}{h_{i}} - \frac{1}{2})u_{i}^{n,0} \right)
\]

\[
+ \frac{1}{2} u_{i}^{n,0} - \frac{1}{2} u_{i}^{n,0} - (\frac{2\lambda_{i}}{h_{i}} - \frac{1}{2})u_{i}^{n,1} + \frac{1}{\lambda_{i}} \left( \frac{1}{2} f_{i}^{n+1} + \frac{1}{2} f_{i}^{n+1} \right)
\]

\[
+ \frac{1}{2} u_{i}^{n,0} - \frac{1}{2} u_{i}^{n,0} - (\frac{2\lambda_{i}}{h_{i}} - \frac{1}{2})u_{i}^{n,1} + \frac{1}{\lambda_{i}} \left( \frac{1}{2} f_{i}^{n+1} + \frac{1}{2} f_{i}^{n+1} \right)
\]

\[
+ \frac{1}{2} u_{i}^{n,0} - \frac{1}{2} u_{i}^{n,0} - (\frac{2\lambda_{i}}{h_{i}} - \frac{1}{2})u_{i}^{n,1} + \frac{1}{\lambda_{i}} \left( \frac{1}{2} f_{i}^{n+1} + \frac{1}{2} f_{i}^{n+1} \right)
\]

\[
+ \frac{1}{2} u_{i}^{n,0} - \frac{1}{2} u_{i}^{n,0} - (\frac{2\lambda_{i}}{h_{i}} - \frac{1}{2})u_{i}^{n,1} + \frac{1}{\lambda_{i}} \left( \frac{1}{2} f_{i}^{n+1} + \frac{1}{2} f_{i}^{n+1} \right).
\]
We are going to impose boundary conditions such that the right-hand side in the previous difference is equal to the difference between the fluxes at the outer boundaries.

Then, we approximate the relation (7) with an implicit-explicit discretization in order to maintain the order of the scheme high, and, using the trapezoidal rule we can write:

$$
I_{tot}^{n+1} - I_{tot}^n = \frac{k}{2} (v_{l}^{n,0} - v_{m}^{n,M,m+1} + v_{l}^{n+1,0} - v_{m}^{n+1,M,m+1})
$$

and then, splitting the terms, for the left boundary (on arc $l$) and right boundary (on arc $m$), we get, respectively,

$$
\frac{k}{2} (w^{n,0} + w^{n+1,0})
= \frac{h_l k}{2} \left( \frac{1}{k} (u_{+l}^{n+1,0} - u_{+l}^{n,0}) + \frac{1}{k} (u_{-l}^{n+1,0} - u_{-l}^{n,0}) + (2\lambda_l h_l - \frac{1}{2}) u_{+l}^{n,0} \right)
+ \frac{1}{2} u_{l}^{n,0} - \frac{1}{2} u_{+l}^{n,1} - \left( 2\Lambda_l h_l - \frac{1}{2} \right) u_{l}^{n,1} + \frac{1}{\Lambda_l} \left( \frac{1}{2} f_l^{n,1} + \frac{1}{2} f_l^{n,0} \right)
$$

(21)

and

$$
\frac{k}{2} (z_{M,m}^{n,M,m+1} + z_{n+1,M,m+1})
= \frac{h_m k}{2} \left( \frac{1}{k} (u_{+m}^{n+1,M,m+1} - u_{+m}^{n,M,m+1}) + \frac{1}{k} (u_{-m}^{n+1,M,m+1} - u_{-m}^{n,M,m+1}) + \frac{1}{2} u_{,+m}^{n,M,m+1} \right)
+ (2\lambda_m h_m - \frac{1}{2}) u_{-m,M,m+1} - \left( 2\Lambda_m h_m - \frac{1}{2} \right) u_{-m,M,m} - \frac{1}{\Lambda_m} \left( \frac{1}{2} f_m^{n,M,m+1} + \frac{1}{2} f_m^{n,M,m} \right)
$$

(22)

Let us now focus on the condition for arc $l$. Making some simplifications and reorganizing the terms in (21) we can rewrite the formula as

$$
w^{n+1,0} =
- w^{n,0} + h_l \left( \frac{1}{k} (u_{+l}^{n+1,0} - u_{+l}^{n,0}) + \frac{1}{k} (u_{-l}^{n+1,0} - u_{-l}^{n,0}) + (2\lambda_l h_l - \frac{1}{2}) u_{+l}^{n,0} \right)
+ \frac{1}{2} u_{l}^{n,0} - \frac{1}{2} u_{+l}^{n,1} - \left( 2\Lambda_l h_l - \frac{1}{2} \right) u_{l}^{n,1} + \frac{1}{\Lambda_l} \left( \frac{1}{2} f_l^{n,1} + \frac{1}{2} f_l^{n,0} \right)
$$

(23)
Then, we separate the terms computed at time $t_{n+1}$ from those computed at $t_n$:

$$
w^{n+1,0} - \frac{h_t}{k}(u_{n+1,0}^{+} + u_{n+1,0}^{-}) = -w^{n,0} + h_t \left( -\frac{1}{k}(u_{n+1,t}^{+} + u_{n+1,t}^{-}) + \left( 2\frac{\lambda_t}{h_t} - \frac{1}{2} \right) u_{n+1,t}^{+} \\
+ \frac{1}{2}u_{n+1,t}^{-} - \frac{1}{2}u_{n+1,t}^{+} - \left( 2\frac{\lambda_t}{h_t} - \frac{1}{2} \right) u_{n+1,t}^{+} + \frac{1}{2} \left( \frac{1}{2}f_{n+1,t}^{+} + \frac{1}{2}f_{n+1,t}^{-} \right) \right). \tag{24}
$$

The computation of the condition above obviously depends on the type of inflow condition $w^{n+1,0}$. In particular, from now on we consider the inflow condition used in the experiments reported in Section 4, namely $v_t^{n+1,0} = w^{n+1,0} = \frac{1}{1 + u_{n+1,i}^{+} + u_{n+1,i}^{-}}$. Let us introduce a parameter $A^n$ to include the terms in (24) depending on $t_n$:

$$
A^n = -\frac{2}{1 + \frac{k}{2}u_{n+1,t}^{+} + u_{n+1,t}^{-}} + h_t \left( -\frac{1}{k}(u_{n+1,t}^{+} + u_{n+1,t}^{-}) + \left( 2\frac{\lambda_t}{h_t} - \frac{1}{2} \right) u_{n+1,t}^{+} \\
+ \frac{1}{2}u_{n+1,t}^{-} - \frac{1}{2}u_{n+1,t}^{+} - \left( 2\frac{\lambda_t}{h_t} - \frac{1}{2} \right) u_{n+1,t}^{+} + \frac{1}{2} \left( \frac{1}{2}f_{n+1,t}^{+} + \frac{1}{2}f_{n+1,t}^{-} \right) \right), \tag{25}
$$

and, set $\alpha_1 = \frac{h_t}{k}$, so that formula (24) becomes:

$$
\frac{2}{1 + \frac{k}{2}u_{n+1,t}^{+} + u_{n+1,t}^{-}} - a_1(u_{n+1,t}^{+} + u_{n+1,t}^{-}) = A^n, \tag{26}
$$

and, with simple computation, one gets:

$$
\alpha_1^{n+1,0} + \left( 2\alpha_1 u_{n+1,t}^{-} \right)^{n+1,0} + \left( \gamma_1^n + \left( \alpha_1(1 + u_{n+1,t}^{-}) + A^n \right) \right) = 0, \tag{27}
$$

with $\beta_1^n = \alpha_1 + A^n$, and $\gamma_1^n = A^n - 2$. Then, choosing the positive root of equation (27), we get the formula:

$$
u_{n+1,i}^{+} := g_1^n(u_{n+1,i}^{-}) = \frac{1}{2\alpha_1} \left[ -\beta_1^n - 2\alpha_1 u_{n+1,i}^{-} \right. \\
+ \left. \left( \beta_1^n + 2\alpha_1 u_{n+1,i}^{-} \right)^2 - 4\alpha_1 \left( \gamma_1^n + u_{n+1,i}^{-} \beta_1^n + \alpha_1(1 + u_{n+1,i}^{-}) \right) \right], \tag{28}
$$

with the radicand positive under the condition $(\beta_1^n)^2 - 4\alpha_1 \gamma_1^n > 0$, which needs to be verified at each time step. We compute (28) using the value of $u_{n+1,i}^{-}$ obtained from the numerical scheme (14) at the boundary $i = 0$.

For the discretization of $f$, we have:

$$
f_t^{n,0} = \chi u_t^{n,0} \phi_x^{n,0},
$$
where $\phi_{x,l}$ is discretized as described in paragraph 3.2, and

$$f_{l}^{n,1} = \chi u_{l}^{n,1} \phi_{x,l}^{n,1} = \chi u_{l}^{n,1} \frac{\phi_{l}^{n,0} - \phi_{l}^{n,0}}{2h_{l}}.$$

Then, plugging the expression above into (14) and denoting $u_{+,-l}^{n+1,0} = g_{l}^{1}(u_{-l}^{n,0})$, we have that the scheme at the left endpoint of arc $l$ is:

$$u_{-l}^{n+1,0} = u_{-l}^{n,0} \left( 1 - \frac{\lambda_{l} k}{h_{l}} - \frac{k}{4} - \frac{k}{4\lambda_{l}} \chi \phi_{n,0}^{x,l,1} + g_{l}^{n-1}(u_{-l}^{n,0}) \left( \frac{k}{4} - \frac{k}{4\lambda_{l}} \chi \phi_{n,0}^{x,l,1} \right) \right).$$

(29)

Reasoning as above, for arc $m$ having an inflow condition $v_{m}^{n+1,M_{m+1}} = z_{m}^{n+1,M_{m+1}} = \frac{1 + u_{+,-m}^{n+1,M_{m+1}} + u_{+,-m}^{n+1,M_{m+1}}}{2}$, we obtain that the scheme at the right endpoint of arc $m$ is:

$$u_{+,-m}^{n+1,0} = u_{+,-m}^{n,0} \left( 1 - \frac{\lambda_{m} k}{h_{m}} - \frac{k}{4} - \frac{k}{4\lambda_{m}} \chi \phi_{n,m+1}^{x,m} + g_{m}^{n-1}(u_{+,-m}^{n,0}) \left( \frac{k}{4} - \frac{k}{4\lambda_{m}} \chi \phi_{n,m+1}^{x,m} \right) \right).$$

(30)

Lemma 1. Under the CFL condition given in [4], namely

$$h_{i} = 2k\lambda_{i},$$

(31)

the scheme at the outer boundaries is monotone if the time step satisfies the condition:

$$k \leq 1,$$

(32)

provided that

$$-1 < \frac{\chi}{\lambda_{l}} \phi_{n,0}^{x,l,1} \leq 1$$

(33)

holds true for (29), and

$$-1 \leq \frac{\chi}{\lambda_{m}} \phi_{n,M_{m}}^{x,m} < 1$$

(34)

holds true for (30).

Remark 3. Note that condition (32) is a sort of subcharacteristic condition. However, the scheme is not monotone in general, since the chemotaxis model itself is not. Indeed, in [4] we investigated the blow-up of solutions occurring
for increasing values of $\phi_x$ during chemotactic process if the mass grows. Note that, this may also cause the $u$ to become negative. Then, at each time step we need to check if the condition (33) is satisfied, in order to have a finite solution.

**Proof.** In order to ensure the monotonicity of the scheme (29), we have to guarantee the coefficients in (29), to be non-negative:

$$
\begin{align*}
\left\{ \begin{array}{l}
\frac{\lambda_l k}{h_t} - \frac{k}{4} - \frac{k \chi}{4 \lambda_l} \phi_{x,l}^{n,1} 
\geq 0, \\
\frac{k}{4} - \frac{k \chi}{4 \lambda_l} \phi_{x,l}^{n,1} 
\geq 0,
\end{array} \right.
\end{align*}
$$

(35)

and we also have to guarantee the monotonicity with respect to $u_{n,l}^{n,0}$ of the first two terms on the right-hand side of equation (29):

$$
u_{n,l}^{n,0} \left( 1 - \frac{\lambda_l k}{h_t} - \frac{k}{4} - \frac{k \chi}{4 \lambda_l} \phi_{x,l}^{n,0} \right) + g_1^{n-1}(u_{n,l}^{n,0}) \left( \frac{k}{4} - \frac{k \chi}{4 \lambda_l} \phi_{x,l}^{n,0} \right).
$$

(36)

With simple computations and using (31) one can rewrite (35) as:

$$
\begin{align*}
\left\{ \begin{array}{l}
2 - k \left( 1 + \frac{\chi}{\lambda_l} \phi_{x,l}^{n,1} \right) 
\geq 0, \iff k \leq \frac{2}{1 + \frac{\chi}{\lambda_l} \phi_{x,l}^{n,1}} \\
\left( 1 - \frac{\chi}{\lambda_l} \phi_{x,l}^{n,1} \right) 
\geq 0, \iff \frac{\chi}{\lambda_l} \phi_{x,l}^{n,1} \leq 1,
\end{array} \right.
\end{align*}
$$

(37)

thus leading to condition $k \leq 1$. Similarly, for the scheme (30), we need to study the conditions:

$$
\begin{align*}
\left\{ \begin{array}{l}
\frac{k}{4} + \frac{k \chi}{4 \lambda_m} \phi_{x,m}^{n,M_m} 
\geq 0, \\
\frac{\lambda_m k}{h_m} - \frac{k}{4} + \frac{k \chi}{4 \lambda_m} \phi_{x,m}^{n,M_m} 
\geq 0,
\end{array} \right.
\end{align*}
$$

(38)

and, proceeding as above in order to have non-negative coefficients we find conditions $k \leq 1$ and (34). Now we discuss the monotonicity with respect to $u_{n,l}^{n,0}$ of the first two terms on the right-hand side of equation (29). Setting $u_{n,l}^{n,0} = u$ in (36) and passing to the derivative respect to $u$, we study the expression

$$
\left( 1 - \frac{\lambda_l k}{h_t} - \frac{k}{4} - \frac{k \chi}{4 \lambda_l} \phi_{x,l}^{n,0} \right) + (g_1^{n-1})'(u) \left( \frac{k}{4} - \frac{k \chi}{4 \lambda_l} \phi_{x,l}^{n,1} \right) \geq 0.
$$

(39)

Deriving $g_1^{n-1}$ we have

$$
\frac{dg_1^{n-1}(u)}{du} =
\frac{1}{2\alpha_1} \left( -2\alpha_1 + \frac{4\alpha_1 (\beta_1^{n-1} - \alpha_1 - A^{n-1})}{2(\beta_1^{n-1} + 2\alpha_1 u)^2 - 4\alpha_1 (\gamma_1^{n-1} + u(A^{n-1} + \alpha_1) + \alpha_1 u^2)} \right).
$$
and, using that $\beta_1^{n-1} = \alpha_1 + A^{n-1}$, we get
\[
\frac{d\phi_i^{n-1}(u)}{du} = -1,
\]
then, under the condition (31), (39) reduces to \( k \leq 1 \), as stated in (32).

Analogously, setting $u^{n,M+1}_{n,m} = u$ in (30), and proceeding as above, we need to study the expression
\[
\left(1 - \frac{\lambda m k}{h_m} - \frac{k}{4} - \frac{k}{4\lambda_m} \chi \phi_{x,m}^{n,M+1}\right) + (g_2^{n-1})' (u) \left(\frac{k}{4} + \frac{k}{4\lambda_m} \chi \phi_{x,m}^{n,M+1}\right) \geq 0.
\]
And, we have again
\[
\frac{d\phi_i^{n-1}(u)}{du} = -1
\]
so that, under the condition (31), (40) reduces to \( k \leq 1 \).

### 3.2. Approximation of the parabolic equation for $\phi$.

As in [4], we solve the parabolic equation, using a finite differences scheme in space and a Crank-Nicolson method in time, namely an explicit-implicit method in time. Respect to [4], here the boundary conditions are written with a more general formula, in order to deal with a general flux of chemoattractant also varying in time at the boundary. We discretize $\phi_{x,i}$ using a second order approximation on each arc $i$. In particular, we use the following discretization, already described in [4], at internal space nodes:
\[
\phi_i^{n+1,j} = \frac{1}{2h_i} \left( \phi_i^{n+1,j+1} - \phi_i^{n+1,j-1} \right), 1 \leq j \leq M_i.
\]

Furthermore, we give a more general formula, respect to that described in [4], for the second order discretization of $\phi_{x,i}$ at the initial and final endpoints connected to outer junctions:

\[
\begin{align*}
\phi_i^{n+1,0} &= \frac{4}{3} \phi_i^{n+1,1} - \frac{1}{3} \phi_i^{n+1,2} - \frac{2h_i}{3} \phi_i^{n+1}, \quad \text{if } i \in O_{\text{out}}, \\
\phi_i^{n+1,M_i+1} &= \frac{4}{3} \phi_i^{n+1,M_i} - \frac{1}{3} \phi_i^{n+1,M_i-1} + \frac{2h_i}{3} \phi_i^{n+1}, \quad \text{if } i \in I_{\text{out}}.
\end{align*}
\]

Note that (41) can be used for any given $\overline{\phi}_i(t)$ as in (6), also including the zero flux case. Moreover, the numerical condition, corresponding to non-constant Neumann boundary conditions (6) in the case $\beta = 1$ and $\overline{\phi}_i(t) = 0$ is as follows:

\[
\begin{align*}
\phi_i^{n+1,0} \left(1 + \frac{2h_i}{3}\right) &= \frac{4}{3} \phi_i^{n+1,1} - \frac{1}{3} \phi_i^{n+1,2}, \quad \text{if } i \in I_{\text{out}}, \\
\phi_i^{n+1,M_i+1} \left(1 - \frac{2h_i}{3}\right) &= \frac{4}{3} \phi_i^{n+1,M_i} - \frac{1}{3} \phi_i^{n+1,M_i-1}, \quad \text{if } i \in O_{\text{out}}.
\end{align*}
\]

**Remark 4.** Here we just give the expression of boundary conditions for an outer node, since the transmission conditions have been already described in [4]. Note that in the case of a constant value at the boundaries, in the...
formula (41) we have \( \tilde{\phi}^n_{i+1} = \tilde{\phi}_i \). In this way we also include null flux condition case considered in our previous work.

In order to compute \( \phi^n_{i+1} \) we need to solve a large system which contains also the discretizations of transmission and boundary conditions.

Here we detail the shape of the sparse matrix of the system. In order to consider any network geometry we need to write an algorithm that takes into account the connections between the arcs. For a network of \( N \) arcs, we need to solve the system \( M \phi^n_{i+1} = c \), with \( c \) the right hand side to be specified later on, and \( M \) the matrix of size \( M_{tot} \times M_{tot} \), with \( M_{tot} = \sum_{i=1}^{N} M_i + 2N \):

\[
M = \begin{bmatrix}
M_1 & & \\
& \ddots & \\
& & M_N
\end{bmatrix}.
\]

In particular, for each arc \( i \) we define the rectangular matrices \( \widetilde{M}_i \) and \( M_i \), both of size \( (M_i + 2) \times M_{tot} \):

\[
\widetilde{M}_i = \begin{pmatrix}
-1 & 2 & -1 & (0) \\
\vdots & \ddots & \ddots & \ddots \\
(0) & -1 & 2 & -1 \\
v_{\text{right}, i}
\end{pmatrix},
\]

\[
M_i = \left( 1 + \frac{b_i k}{2} \right) I + \frac{k}{2h_i^2} D_i \widetilde{M}_i.
\]

Note that the vectors \( v_{\text{left}, i} \) and \( v_{\text{right}, i} \) have length \( M_{tot} \) and describe the left and right boundaries of arc \( i \). We recall that, as in [4], for an arc \( i \) outgoing from node \( p_1 \) and connected to \( j \) arcs we set \( \eta_{\text{in}}^i = 1 + \frac{2h_i}{3} \sum_{j \in I_{p_1} \cup O_{p_1}} \kappa_{i,j} \) and analogously, we define \( \eta_{\text{out}}^i \) if the arc is incoming in node \( p_2 \) and is and connected to \( j \) arcs. Moreover, for an arc linked with a outer node in the case of condition (6) with \( \beta = 0 \) or in case of homogeneous boundary condition we have \( \eta_{\text{out}}^i = 1 \), otherwise, in case of condition (6) with \( \beta = 1 \) and \( \tilde{\phi}_i(t) = 0 \) we have \( \eta_{\text{out}}^i = 1 + 2h_i/3 \) at \( j = 0 \) corresponding to left boundary or \( \eta_{\text{out}}^i = 1 - 2h_i/3 \) at \( j = M_i + 1 \) corresponding to right boundary. If arc \( i \) is connected on the left with an arc \( j \), we have to take it into account into the vector \( (v_{\text{left}, i})_l \), at the index indicated by label \( l \in \{1, \ldots, M_{tot} \} \), in order to couple the \( \phi \) functions of arcs having a node in common. Analogously, for an arc connected on the right, we insert the coupling condition at the index \( (v_{\text{right}, i})_l \), \( l \in \{1, \ldots, M_{tot} \} \). Let us consider, for instance, the network in Figure 1. In this case we have that the vectors
of length $M_{tot} = \sum_{i=1}^{3} M_i + 6$, are:

\[
v_{\text{left}, 1} = (\eta_{1}^{\text{out}}, -4/3, 1/3, 0, \ldots, 0),
\]

\[
v_{\text{right}, 1} = (0, \ldots, 0, 1/3, 4/3, \eta_{1}^{1} = 1 + \frac{2 h_{1}}{3 D_{1}} (\kappa_{1,2} + \kappa_{1,3}),
\]

\[
- \frac{2 h_{1}}{3 D_{1}} \kappa_{1,2}, 0, \ldots, 0 \bigg|_{l=M_1+3} - \frac{2 h_{1}}{3 D_{1}} \kappa_{1,3}, 0, \ldots, 0 \bigg|_{l=M_1+M_2+5},
\]

\[
v_{\text{left}, 2} = (0, \ldots, 0, -\frac{2 h_{2}}{3 D_{2}} \kappa_{2,1}, \eta_{2}^{1} = 1 + \frac{2 h_{2}}{3 D_{2}} (\kappa_{2,1} + \kappa_{2,3}),
\]

\[
- \frac{2 h_{2}}{3 D_{2}} \kappa_{2,3}, 0, \ldots, 0 \bigg|_{l=M_1+3} - \frac{2 h_{2}}{3 D_{2}} \kappa_{2,3}, 0, \ldots, 0 \bigg|_{l=M_1+M_2+5},
\]

\[
v_{\text{right}, 2} = (0, \ldots, 0, 1/3, 4/3, \eta_{2}^{\text{out}}, 0, \ldots, 0),
\]

\[
v_{\text{left}, 3} = (0, \ldots, 0, -\frac{2 h_{3}}{3 D_{3}} \kappa_{3,1}, -\frac{2 h_{3}}{3 D_{3}} \kappa_{3,2}, \ldots, 0,
\]

\[
\eta_{3}^{1} = 1 + \frac{2 h_{3}}{3 D_{3}} (\kappa_{3,1} + \kappa_{3,2}), -4/3, 1/3, 0, \ldots, 0, \bigg|_{l=M_1+M_2+5},
\]

\[
v_{\text{right}, 3} = (0, \ldots, 0, 1/3, 4/3, \eta_{3}^{\text{out}}),
\]

\[
\bigg|_{l=M_{tot}}.
\]

Note that, as already mentioned in Section 2, $\kappa_{i,j} = \kappa_{j,i}, i, j = 1, 2, 3$, to have the conservation of fluxes at the junction. Now we give the expression, in the general case, of the vector on right hand side $c$, having length $M_{tot}$. We have

\[
c = (c_1, \ldots, c_N)^T,
\]

with each component of the vector given by the subvector $c_i$ corresponding to the arc $i = 1, \ldots, N$:

\[
c_i = (c_{i,0}, c_{i,1}, \ldots, c_{i,M_i}, c_{i,M_i+1})^T.
\]

Let us detail the components $c_{i,j}, j = 0, \ldots, M_i + 1$. For the indexes $j = 1, \ldots, M_i$, describing the inner space nodes of the arc $i$, we have:

\[
c_{i,j} = \left( 1 - \frac{D_i k}{h_i^2} \right) \phi_i^{n,j} - \frac{D_i k}{2 h_i^2} (-\phi_i^{n,j+1} - \phi_i^{n,j-1}) + \frac{a_{i,k}}{2} (u_i^{n+1,j} + u_i^{n,j}) - \frac{b_{i,k}}{2} \phi_i^{n,j},
\]

\[
\bigg|_{l=M_{tot}}.
\]
while the first and the last component, respectively \( c_{i,0} \) and \( c_{i,M_i+1} \), include the discretization of boundary conditions (6). Let us consider for example the boundary of an arc connected to an outer node on the left. If \( \phi_i(t) \) is independent of \( \phi_i(0,t) \), we have:

\[
c_{i,0} = -\frac{2h_i}{3} \bar{\phi}_i^{n+1},
\]

while, in the case of homogeneous boundary conditions or condition (6) with \( \phi_i(t) = 0 \) we have \( c_{i,0} = 0 \). Analogously, for the boundary condition of an arc connected to an outer node on the right, if \( \phi_i(t) \) is independent of \( \phi_i(L_i,t) \), we have:

\[
c_{i,M_i+1} = \frac{2h_i}{3} \bar{\phi}_i^{n+1},
\]

while, in the case of homogeneous boundary conditions or condition (6) with \( \phi_i(t) = 0 \) we have \( c_{i,M_i+1} = 0 \).

For the computational resolution of the system we used the LAPACK-Linear Algebra PACKage routine DGBSV designed for banded matrix. Once the values of \( \phi_i^{n+1,j} \) are known, we can compute a second-order discretization of the derivatives \( \phi_i^{n+1,j,x} \) as described above.

4. Tests on different network geometries. Here we present some computational tests on different network topologies to investigate the behaviour of individuals moving through them. We firstly consider the basic network composed of one incoming and two outgoing arcs (T-shaped network) in order to show that the model is able to reproduce the main features of the plasmodium. Then we consider a network of 7 arcs and 6 nodes (diamond-like graph) and a more complex network of 26 arcs and 18 nodes, both of them connecting two exits (a source and a sink), where inflow conditions are implemented to mimic the presence of food sources. Finally, we consider a network of 21 arcs and 15 nodes with multiple exits (two sources and three sinks).

For all the networks we deal with we assume to have equal velocities \( \lambda_i = \lambda \) and equally distributed transmission coefficients at each node. If, for instance, we have a node \( p \) connected with the total number of \( N \) arcs (no matter how many are incoming or outgoing), we assume to have:

\[
\xi_{ij} = \frac{1}{N}, \forall i \in I_p, \forall j \in O_p.
\] (43)

It is easy to verify that setting transmission coefficients as in (43) allows to satisfy both the conditions (10) and (11). For a more detailed study on the choice of transmission coefficients connected with the energy dissipation property of the hyperbolic part of the system without the source term on a general network, see [4].
4.1. T-shaped graph: four nodes and three edges. Here we consider the network of three arcs and four nodes (1 internal node and three external nodes) shown in Figure 1. We assume to have arcs of length $L_i = 1$ and we set parameters as $a_i = 1, b_i = 0.1, \lambda_i = \sqrt{0.33}, D_i = 1$, with $\chi_i = 1$ representing positive chemotaxis, for $i = 1, 2, 3$. Furthermore, for the transmission conditions for $u$ at the internal node we set dissipative coefficients $\xi_{i,j} = \frac{1}{3}$ for $i, j = 1, 2, 3$ and for the transmission conditions for $\phi$ we assume $\kappa_{i,j} = 1$ for $i \neq j$ and $\kappa_{i,i} = 0$, for $i, j = 1, 2, 3$.

4.1.1. T-shaped graph. Here, starting from the experiment with the T-shaped plasmodium tubes of Physarum presented in [25], we aim at showing the property of dead-end cutting. Therefore, we set non-homogeneous Neumann boundary conditions at the outer boundaries for $\phi$, to mimic the presence of food at the left and lower ends, namely:

$$
\partial_x \phi_1(0, t) = -1, \quad \partial_x \phi_2(L_2, t) = 1.
$$

(44)

For $u$ we impose homogeneous Neumann boundary conditions at the outer boundaries. The initial values for $u_i$ are randomly equally distributed in $[0.25, 0.35]$ for each $i = 1, 2, 3$ to mimic the plasmodium spread in the network, while we set $\phi_i(x, 0) = 0, i = 1, 2, 3$.

Let us recall that in our modeling the dead-end cutting property corresponds to have a mass equal to zero on the edges where the flux is null. In accordance to the cited experiment, as the organism starts moving to feed itself, we observe that the mass concentrate on the left and lower edges (arcs 1 and 2) since food sources are located at the outer nodes 0 and 2, see Figures 2 and 3. The mass decreases quickly until it becomes null on the upper edge (arc 3), whose endpoint has no food source, see Figures 4 and 5. Note that the solution reached at time $T = 20$ is stationary up to an accuracy of $10^{-7}$ on $u, v$ and $5 \times 10^{-5}$ on $\phi$.

For completeness, we investigated the speed of convergence to get the stationary solution, with a threshold of $10^{-5}$ for the accuracy of the solutions on $u, v$, and $\phi$, as a function of the speed $\lambda$ and as a function of the length of the arcs $L$. We noticed that the final time $T_f$ is approximately constant as a function of $\lambda$. On the contrary, if we change $L$ keeping the total mass fixed, the speed of convergence grows both for $L$ decreasing and for $L$ increasing. This can be explained in this way: when $L$ is small there is a slow diffusion regime dominating in the evolution process, thus the equilibrium of the parabolic equation is reached slowly; on the contrary, when $L$ is high, there is an hyperbolic regime dominating, so that the parabolic equation reaches fast the equilibrium, while $u$ and $v$ are still evolving to reach the equilibrium. We do not report the graph in the paper to not make it too long.
Figure 1. Network of three edges: one incoming and two outgoing arcs (T-shaped network).
Figure 2. T-shaped graph. The distribution of the density of cells on the T-shaped network at time $t = 1$, with homogeneous Neumann boundary conditions on $u$ and conditions (44) on $\phi$. 
Figure 3. T-shaped graph. The distribution of the density of cells on the T-shaped network at time $t = 3$, with homogeneous Neumann boundary conditions on $u$ and conditions (44) on $\phi$. 
Figure 4. T-shaped graph. The distribution of the density of cells on the T-shaped network at time \( t = 6 \), with homogeneous Neumann boundary conditions on \( u \) and conditions (44) on \( \phi \).
Figure 5. T-shaped graph. The distribution of the density of cells on the T-shaped network at time $t = 20$, with homogeneous Neumann boundary conditions on $u$ and conditions (44) on $\phi$. 
4.2. **Study on the path followed by amoeboid-like organism.** Here we are interested in the identification of the shortest path followed by individuals in the case of positive (attractive) chemotaxis.

4.2.1. **Wheatstone bridge-shaped network with a source and a sink (two exits).** Let us consider the Wheatstone bridge-shaped network where, for our convenience, we inserted one incoming and one outgoing arc, respectively, exiting or entering an external node, as shown in Fig. 6. Since this modification does not change the structure of the shortest paths in the network, the analysis on the Wheatstone bridge network can be found in [18], where it was proved that the globally asymptotically stable equilibrium point corresponds to the shortest path connecting the exits.

If, for instance, we want the path $1 \rightarrow 2 \rightarrow 6 \rightarrow 4 \rightarrow 7$ to be shortest one, we need to set:

$$L_2 + L_6 < L_5 \text{ and } L_4 + L_6 < L_3. \quad (45)$$

In particular, we assume

$$L_1 = L_7 = 0.2, \ L_2 = L_4 = 0.3, \ L_3 = L_5 = 2, \ L_6 = 0.3.$$ 

Note that in Fig. 6 we depicted the arcs composing the shortest path with the dashed line.

We set parameters as $a_i = 1, b_i = 0.1, \lambda_i = \sqrt{0.33}, \chi_i = 1, \ D_i = 1$, for $i = 1, \ldots, 7$. As before, for the transmission conditions for $u$, at each node $p$ we set dissipative coefficients $\xi_{i,j} = \frac{1}{3}$ for $i, j = 1, \ldots, 7$ and for the transmission conditions for $\phi$ we assume $\kappa_{i,j} = 1$ for $i \neq j$ and $\kappa_{i,i} = 0$, for $i, j = 1, \ldots, 7$.

The initial values for $u_i$ are randomly equally distributed in $[0.45, 0.55]$ and we set $\phi_i(x, 0) = 0$ for each $i = 1, \ldots, 7$.

We set non-homogeneous Neumann boundary conditions for the chemottractant $\phi$ at the node 0 and at the node 5 (inflow conditions):

$$\partial_x \phi_1(0, t) = -1, \quad \partial_x \phi_7(L_7, t) = 1. \quad (46)$$

Firstly, at the outer boundaries we assume homogeneous Neumann conditions $u_x(\cdot, t) = 0$ corresponding to $v_1(0, t) = 0$ and $v_7(L_7, t) = 0$.

The effect on the movement of the organism is that it is able to find the shortest path connecting node 0 with node 5 in such a way to minimize the sum of the length of the arcs composing the path. As a result, see Figures 7-8-9-10, the mass concentration is higher on the arcs composing the shortest path, as underlined by the colourscale and thickness of the line connecting nodes. Note that the solution obtained at time $T = 6$ is a stationary state.
Then, to have a certain quantity of cells enters into the network by the node 0 and the node 5, we set non-zero flux conditions at the outer boundaries (19) at the node 0 and (20) at the node 5:

\[
v_1(0, t) = \frac{2}{1 + u_1(0, t)}, \quad v_7(L_7, t) = -\frac{2}{1 + u_7(L_7, t)}. \tag{47}
\]

As in the previous case, cells migrate on the arcs on the shortest path connecting node 0 with node 5 in such a way to minimize the sum of the length of the arcs composing the path. As shown in the following Figures 11-12-13-14, the mass concentration is higher on the path of minimum total length. In this case the connection between the two exits is more evident, as underlined by the range of the density in the colourscale.
Figure 7. Wheatstone bridge-shaped network. The distribution of the density on the diamond graph-like network at time 0.5, with homogeneous Neumann boundary conditions on $u$ and conditions (46) for $\phi$.

4.2.2. A network with two exits: the maze. Inspired by the experiment on ph ysarum in [21] and by numerical simulations in [3], the network considered here is a maze composed of 26 arcs and 18 nodes, with the exits placed at the node 0 (source) and at the node 17 (sink). We set the length $L_i = 0.5$ on arcs $i = 1, 5, 9, 10, 14, 21, 25, 26$ and $L_i = 10$ on the others. Note that in Figure 15 we represent such network, with the shortest arcs depicted with the straight line and the longest arcs with the curve line.
We set parameters as $a_i = 1, b_i = 0.1, \lambda_i = \sqrt{0.33}, D_i = 1, \chi_i = 1$, for all $i$, considering again positive chemotaxis. Furthermore, for the transmission conditions for $u$ we set dissipative coefficients $\xi_{i,j}$, see Table 1, and for the transmission conditions on $\phi$ we assume again $\kappa_{i,j} = 1$ for $i \neq j$ and $\kappa_{i,i} = 0$, for $i, j = 1, \ldots, 26$. The initial values for $u_i$ are randomly equally distributed in $[0.45, 0.55]$ and we assume $\phi_i(x, 0) = 0, \forall i$.

Table 1. Transmission coefficients used for the numerical simulations of the maze in Fig. 15 given node by node.

<table>
<thead>
<tr>
<th>node $p$</th>
<th>$\xi_{i,j}$</th>
<th>$\xi_{i,j}$</th>
<th>$\xi_{i,j}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>p= 1, 2, 3, 5, 8, 9, 12, 14, 15, 16</td>
<td>$\xi_{i,j} = \xi_{i,j}$</td>
<td>$\xi_{i,j} = \xi_{i,j}$</td>
<td>$\xi_{i,j} = \xi_{i,j}$</td>
</tr>
<tr>
<td>p= 4, 13</td>
<td>$\xi_{i,j} = \xi_{i,j}$</td>
<td>$\xi_{i,j} = \xi_{i,j}$</td>
<td>$\xi_{i,j} = \xi_{i,j}$</td>
</tr>
<tr>
<td>p= 6, 7, 10, 11</td>
<td>$\xi_{i,j} = \xi_{i,j}$</td>
<td>$\xi_{i,j} = \xi_{i,j}$</td>
<td>$\xi_{i,j} = \xi_{i,j}$</td>
</tr>
</tbody>
</table>

Here we set non-homogeneous Neumann boundary conditions at the outer boundaries for $\phi$: inflow conditions leading to a high concentration of the
Figure 9. Wheatstone bridge-shaped network. The distribution of the density on the diamond graph-like network at time $t = 2.5$, with homogeneous Neumann boundary conditions on $u$ and conditions (46) for $\phi$.

Furthermore, to have a certain quantity of cells enters into the network by the node 0 and the node 17, we set non-zero flux conditions at the outer boundaries:

$$v_1(0, t) = \frac{2}{1 + u_1(0, t)}, \quad v_{26}(L_{26}, t) = -\frac{2}{1 + u_{26}(L_{26}, t)}.$$  \hspace{1cm} (49)

The effect on the movement of the cells is that they try to find the minimum-length way connecting node 0 with node 17 in order to minimize the sum of the length of the arcs composing the path. Let us recall that the dead-end cutting of the zones with no-flux and the shortest path selection is here represented, as shown in the following Figures 16-17-18-19, by the higher mass concentration on the edges composing the shortest path. We also observe that at a certain time blow up of solutions verifies, due to the growth
Figure 10. Wheatstone bridge-shaped network. The distribution of the density on the diamond graph-like network at time $t = 6$, with homogeneous Neumann boundary conditions on $u$ and conditions (46) for $\phi$.

of the total mass. We remark that, though the evolution is slower respect to that presented in [3], the results are asymptotically the same obtained in [3]. More in detail, the results obtained in [3] at time 5 are comparable to those obtained here at time $t = 60$. Furthermore, the maximum value of density obtained with the hyperbolic model is higher, as expected, since the process is slower.

The simulation of the network above was performed by a personal computer, processor Intel Centrino core 2 Duo 2 Ghz, RAM 3 Gb and the CPU time for 1333 time iterations was 19.71 s.
Figure 11. Wheatstone bridge-shaped network. The distribution of the density on the diamond graph-like network at time $t = 10$, with non-homogeneous Neumann boundary conditions (47) and (46).

4.2.3. A network with more than two exits. Here we consider a network with more than two exits (NM2E): in fact in this case we have two sources and three sinks. We underline that is the first time that this case is simulated with a chemotaxis PDE model. Moreover, the feeding process in the case of more than two food sources it has not been completely clarified yet by the ODE models describing the dynamics of physarum. To better understand the mechanism of the feeding process in such a case, we consider a network with more than two sources of food and we found that the minimum-path property is maintained, in the sense that the organism traces the path minimizing the sum of the total length of the arcs. More in details, we consider a network composed of 21 arcs and 15 nodes, with the sources placed at the nodes 0 and 1, while the sinks are at the nodes 9, 10 and 11, we set the length $L_i = 0.5$ on arcs $i = 1, 2, 3, 4, 8, 13, 14, 15, 19, 20, 21$ and $L_i = 10$ on the others. The network we consider is shown in Figure 20, where the shortest arcs are depicted with the dashed line.
As before, we set parameters as \( a_i = 1, b_i = 0.1, \lambda_i = \sqrt{0.33}, D_i = 1, \chi_i = 1 \), for all \( i \). Furthermore, for the transmission conditions for \( u \), we set dissipative coefficients \( \xi_{i,j} \), see Table 2, and for the transmission conditions on \( \phi \) we assume \( \kappa_{i,j} = 1 \) for \( i \neq j \) and \( \kappa_{i,i} = 0 \), for \( i, j = 1, \ldots, 21 \). We assume the inflow boundary conditions:

\[
\partial_x \phi_1(0, t) = -1 = \partial_x \phi_2(0, t), \quad \partial_x \phi_{19}(L_{19}, t) = 1 = \partial_x \phi_{20}(L_{20}, t) = \partial_x \phi_{21}(L_{21}, t).
\] (50)

Moreover, we assume for \( u \) homogeneous Neumann boundary conditions \( u_x(\cdot, t) = 0 \) at the nodes 0,1 and at the nodes 9,10,11.
Figure 13. Wheatstone bridge-shaped network. The distribution of the density on the diamond graph-like network at time $t = 130$, with non-homogeneous Neumann boundary conditions (47) and (46).

The initial values for $u_i$ are randomly equally distributed in $[0.45, 0.55]$ and we assume $\phi_i(x, 0) = 0$, $\forall i$.

Even in this case, the organism traces the path connecting nodes 0 and 1 with nodes 19, 20, 21 in such a way to minimize the sum of the total length of the arcs. As a result, see the following Figures 21-22-23-24, besides the arcs connected to the exits (1, 2, 19, 20, 21), the path includes the arcs with minimum length 3, 4, 8, 13, 14, 15.
Figure 14. Wheatstone bridge-shaped network. The distribution of the density on the diamond graph-like network at time $t = 200$, with non-homogeneous Neumann boundary conditions (47) and (46).

5. Conclusion and future perspectives. The main feature of the present work has been the extension of the numerical treatment of system (1) to the case of non-homogeneous boundary conditions, thus resulting in an extension of the AHO scheme to include such a case. With the new scheme it was possible to simulate more different situations at the boundary of the networks considered, in order to better understand the behavior of cells, having in mind the laboratory and theoretical experiments made on physarum for the search of the shortest path. It was also possible to make a comparison with the outcomes presented in the work of Borsche et al. based on a parabolic PDE (KS) model. Differently from KS model, the hyperbolicity of the model (1) allows to have a finite speed of propagation of cells, thus showing a richest dynamics during the observation of cell movements. We also underline that the discontinuity at the junctions of networks is a more realistic condition.

The numerical tests presented in Section 4 show the correspondence between our simulations and the real behavior of slime mold showed through the laboratory experiments. Mainly, we could find that cells move through
the network composing the shortest path while searching for food. The comparison with KS model also show the substantially analogous behavior of cells described by a PDE model, but the feature of the hyperbolic model allow to have a more detailed description of the dynamics of the intermediate states in the cell movements while composing a path. In the future we aim at studying analytically the long time asymptotic behavior for homogeneous boundary conditions.
Figure 16. The maze. The distribution of the density $u_i(x,t)$ on the network in Fig. 15 at time $t = 3$, with non-homogeneous boundary conditions (49) and (48).

REFERENCES

Figure 17. The maze. The distribution of the density $u_i(x,t)$ on the network in Fig. 15 at time $t = 12$, with non-homogeneous boundary conditions (49) and (48).


Figure 18. The maze. The distribution of the density $u_i(x,t)$ on the network in Fig. 15 at time $t = 30$, with nonhomogeneous boundary conditions (49) and (48).

Figure 19. The maze. The distribution of the density $u_i(x,t)$ on the network in Fig. 15 at time $t = 60$, with non-homogeneous boundary conditions (49) and (48).

Figure 20. Network of 21 arcs and 15 nodes (NM2E): the dashed line represents the shortest arcs.
Figure 21. The distribution of the density $u_i(x, t)$ on the network NM2E in Fig. 20 at time $t = 10$, with homogeneous Neumann boundary conditions on $u$ and conditions (50) for $\phi$.


Figure 22. The distribution of the density $u_i(x,t)$ on the network NM2E in Fig. 20 at time $t = 30$, with homogeneous Neumann boundary conditions on $u$ and conditions (50) for $\phi$. 

![Graph](image-url)
Figure 23. The distribution of the density $u_i(x,t)$ on the network NM2E in Fig. 20 at time $t = 60$, with homogeneous Neumann boundary conditions on $u$ and conditions (50) for $\phi$. 
Figure 24. The distribution of the density $u_i(x,t)$ on the network NM2E in Fig. 20 at time $t = 180$, with homogeneous Neumann boundary conditions on $u$ and conditions (50) for $\phi$. 