Discretization of an adaptive prediction model using a non-homogeneous meshing

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ABSTRACT. In a previous work, we have developed a model based on 2D diffusion equations which was discretized on homogeneous meshes taking into account the mobility of entities in an existing prediction model. This model does not fit with the reality of administrative boundaries. The purpose of this paper is to deal with a more realistic approach where the boundary of the study regions are irregular. The work is done in a meshing imposed by the geographical configuration of the administrative divisions and the discretization is done with the finite volumes method for complex geometries. The validation is done using a set of administrative divisions through a multi-agent system and a shapefile extracted in a geographic information system were the modified SIR epidemiological model is applied to highlight the dynamic effect in the spread.

KEYWORDS: Prediction model, Diffusion equation, Complex geometry, discretization, finite volume methods

1. Introduction

The numerical evaluation and implementation of a continuous model is possible through the discretization, which is the first step in the process of transferring the equations into the discrete counterparts [13, 15]. This transformation usually simplify some aspects of the reality as well as it approximates the hypothesis of the models. In the prediction domain like other fields of research, they are some cases where the developed theories do not confirm the reality. In this work we have gone through several prediction model in epidemiology [3, 4, 8, and 9]. The gap between the simulation and the reality of the field is due to the assumption that are made during the transformation of the model. Concerning the domain of complex systems, particularly the prediction of phenomena, the dynamic aspect of mobile entities which are moving in the studied environment is not consider.

In the previous studies [11], a diffusion equation was written to manage the mobility of the entities. Since their displacement is random, a probabilistic matrix was introduced to integrate the adaptation of the model. In the construction of this model, which resulted in 2D diffusion equations, approximations have been made. With all these assumptions, it is clear that the model implemented does not represent the reality reliably then it would be normal that certain results do not comply with the observation as we specified above. Based on these remarks, we come up with the idea of making the model more realistic by first changing the forms of the sites to get closer to the real geographical forms.

The purpose of this article is to improve the discretization of the established model in order to fit closer to reality through the application of this model independently to the geometries of the studied region. To this effect, the initial discrete model obtained with the finite volumes method on regular meshes is modify considering non homogeneous meshes to manage complex geometries. This approach is due to the real configuration of the study sites whose shapes are mainly arbitrary. For illustration, four sites in a real environment are chosen from the administrative divisions through a GIS to constitute a closed environment where simulations will be made.

The rest of this paper is structured as follows. The section 2 presents the literature review where the basic theories and the former development are described. The section 3 presents the methodology, the manner in which the model is built with finite volume discretization for complex geometries. Section 4 describes a hybrid SIR obtained by applying this idea on the traditional SIR model. We will end in section 5 with a conclusion and further works.

2. Background.

2.1. Population dynamics and particles diffusion

The foundation of this study is focused on the equations taken in [7] with the following forms

$$\frac{\partial u(t,x)}{\partial t} = D(u)(t,x) + f(x,u(t,x)) \qquad t > 0, \ x \in R$$
(1)

These equations occur in a wide variety of fields such as combustion, chemistry, biology or ecology. They are used to model the evolution of the entities that interact with each other and move. Applied to the population dynamics, the quantity u(t, x) represents the population density at the period t at the position x. The reaction term f(x, u) corresponds to the growth rate of the population. The movement of individuals is described by the dispersion operator D. Depending on the mode of movement of the individuals, this operator will be local or non-local. Our attention is focused mainly on a single type of reaction-dispersion equation where the dispersion operator D is an elliptic differential operator of the second order.

$$\frac{\partial u(t,x)}{\partial t} = \frac{\partial^2 u(t,x)}{\partial x^2} + f(x,u(t,x))$$
(2)

In this first family of equations we found that the equation of dimension is not valid, equation is purely mathematical but the objective of this work is to deal with the quantities reliable with the reality. This motivated a balance approach that originated in the particles diffusion

In [11] it is found that the equations resulting from the particles diffusion come from the balances of mobile entities in a control volume, this approach was built with the help of [10].

In the same way, [6] starting with the basic concepts developed a model for the spatial spread of diseases involving hosts in random displacement during certain stages of the progression of the disease. It led to a diffusion model based on the conservation law and Fick's law. He applied this model to the study of two cases, namely the spread of rabies in continental Europe during the period 1945-1985 and the rate of spread of West Nile virus in North America.

2.3. The former development

With the basic equation
$$\frac{\partial u(t,x)}{\partial t} = D\left(\frac{\partial^2 u(t,x)}{\partial x^2} + \frac{\partial^2 u(t,y)}{\partial y^2}\right)$$
 (3)

We considered a closed environment with homogeneous site distribution, then the discrete model was suitable. The choice fell on the finite volume discretization method which is adapted to the equations that represent conservation laws [12], [2], [1] and [5]. Then the D coefficient were built according to hypotheses.

The coefficient D is a probabilistic contribution matrix. The general term of D is $D_{i,j} = \omega P_{i,j}$ where $\omega \approx (\Delta x^2)/\Delta t$ depends on the average speed characteristic of the flow moving of mobile entities and $P_{i,j}$ the probabilistic matrix of movements. After applying the finite volume method and assumptions the following numerical scheme were obtained $u_{i,j,k}^{n+1} = \frac{\Delta t D_{l,k}}{\Delta x^2} \left(u_{i+1,j,x}^n \delta_{l,x} + u_{i-1,j,y}^n \delta_{l,y} \right) + \frac{\Delta t D_{l,k}}{\Delta y^2} \left(u_{i,j+1,z}^n \delta_{l,z} + u_{i,j-1,t}^n \delta_{l,t} \right) + (1 - 2(\frac{\Delta t D_{l,k}}{\Delta x^2} + \frac{\Delta t D_{l,k}}{\Delta y^2})) u_{i,j,k}^n \delta_{l,k}$ (4)

3. Methodology of a new approach in real context

The sample regions are approximated by the polygons as shown in Figure 1.



Figure 1. The sample regions and the polygonal approximations

The following considerations are made:

- X_H and X_N are the position of center of gravity of two any regions denoted by (H) and (N)
- |σ_{HN}| the length of the ridge that separates H and N perpendicularly to the line (X_HX_N)
- |*H*| measurement of control volume of the region H
- d_{HN} measurement of the distance $X_H X_N$
- ∂H set of all the outline of any region H

Let remember the basic equation of the model (4)

$$\frac{\partial u(t,x)}{\partial t} = D\left(\frac{\partial^2 u(t,x)}{\partial x^2} + \frac{\partial^2 u(t,x)}{\partial y^2}\right) \leftrightarrow \frac{\partial u(t,x)}{\partial t} = D\Delta u(t,x)$$

u(t, x) represent the number of mobile entities in the site x at the time t. We will look for an approximate value of this number using the previous assumptions. The quantity $\frac{\partial u(t,x)}{\partial t}$ will be approximated by the explicit method of Euler $\frac{\partial u(t,x)}{\partial t} = \frac{u^{n+1}-u^n}{\Delta t}$ (5) u^{n+1} represent the number of mobile entities in the site at the time t + dt and u^n is the value at the period time t.

The finite volume method for complex geometry applied to the basic equation using STOKES' formula [5] in any control volume H, leads to

$$u_H^{n+1} = \sum_{N \in neighbour(H)} D_{NH} |\sigma_{HN}| \Delta t \frac{u_N^n - u_H^n}{|H|d_{HN}} + u_H^n$$
(6)

- u_H^{n+1} represents the number of mobile entities at the time t + dt in H
- $D_{i,j} = \omega P_{i,j}$ represent an element of the diffusion matrix where ω is the average speed of diffusion and $P_{i,j}$ the matrix of random contributions between sites.
- Δt is the time step in the numerical scheme

The boundary conditions are implicitly considered because the quantities above (u^n and u^{n+1}) are zero everywhere else except on the boundaries between our experimental environments.

4. Validation and interpretation

The case study is taken from the epidemiology considering the traditional SIR (Susceptible, Infected, and Retired) model [14]. The diffusion is considered through propagation dynamic of the infection.



Figure 2. Transition state diagram of an individual

Note on the Figure 2 that an individual before being in a Remove state (R) must previously passed through the infected state; and only susceptible individuals can become infected.

Three administratives regions of the Cameroon are concerned in the illustration denoted H, N, P, R as shown in Figure 3.



Figure 3. Polygonal approximation of the selected regions

In the case of the dynamics of the phenomenon taking into account the spatiotemporal dynamics, we have the following discrete equations for the site H knowing that the value u(t, x) is considered for each state S, I, R.

$$\begin{cases} S_{H}^{n+1} = D_{NH} |\sigma_{HN}| \Delta t \frac{S_{N}^{n} - S_{H}^{n}}{|H|d_{HN}} + D_{PH} |\sigma_{PH}| \Delta t \frac{S_{P}^{n} - S_{H}^{n}}{|H|d_{HP}} + S_{H}^{n} + \Delta t (\gamma R_{H}^{n} - \alpha S_{H}^{n}) \\ I_{H}^{n+1} = D_{NH} |\sigma_{HN}| \Delta t \frac{I_{N}^{n} - I_{H}^{n}}{|H|d_{HN}} + D_{PH} |\sigma_{PH}| \Delta t \frac{I_{P}^{n} - I_{H}^{n}}{|H|d_{HP}} + I_{H}^{n} + \Delta t (\alpha S_{H}^{n} - \beta I_{H}^{n}) \\ R_{H}^{n+1} = D_{NH} |\sigma_{HN}| \Delta t \frac{R_{N}^{n} - R_{H}^{n}}{|H|d_{HN}} + D_{PH} |\sigma_{PH}| \Delta t \frac{R_{P}^{n} - R_{H}^{n}}{|H|d_{HP}} + R_{H}^{n} + \Delta t (\beta I_{H}^{n} - \gamma R_{H}^{n}) \\ \text{These equations are replicated for each regions considering its} \end{cases}$$

neighborhood.

4.1. Simulation

The software tool is built on REPAST SYMPHONY which is a multi-agent development environment. The regions are extracted from a GIS, then the corresponding shapefiles are integrated in REPAST. The equations are encoded as the behavior of the agents. The parameters fixed before running the simulation are mentioned in Table 1. Initial parameters of the simulation Table 1.

Table 1. Initial parameters of the simulation

Parameter	Value	Parameters	value
Susceptible agent per region	200	The distance of contamination	500 meters
Infected agent per region	1	The probability of changing the state from I to R	0.2
The number of agents retired	0	The probability of leaving	0.5
per zone		an area	
The probability of changing the state from S to I	0.5		
The probability of changing the state from R to S	0.05		
The diffusion velocity	10km/days		



Figure 4. Infection at the initialization, then after 5, 10 and 20 cycles respectively

4.2. Discussion

Starting from the differential equations of the propagation of an epidemic in SIR model, we obtained a hybrid equations system coupled to the model developed to manage the dynamics of the mobile entities. By analyzing the comparative histogram (see the annexes), the following observations are made:

- High density areas carry the epidemic faster. Having the same number of agents, on all the sites, it is the smallest sites in area which have a high rate of contamination, here: H and K;
- The epidemic persists longer when there is diffusion. This is the case of the region N where the density is low. The epidemic, when there is no diffusion disappears after a few days for lack of contact. Yet the diffusion shows that patients from neighboring areas are reviving the epidemic after the infected natives in the area are cured.
- It can be concluded from the analysis of the data presented that the diffusion of mobile entities has an impact on the life cycle of an epidemiological phenomenon also in the case of complex geometry. This observation validates the hypothesis make at the beginning of this work.

5. Conclusion

The study carried in this paper focus on the discretization on non-homogeneous meshes of an adaptive prediction model built on the basis of diffusion equations. The approach adopted is based on the finite volume method for complex geometries for a mesh imposed by the geometry of the study environment which can be mapped to the administrative division of a territory.

First, it was necessary to recall the basis of the model. Then, the hypothesis were extended to meet the resulting equations from the discretization in a non-homogeneous mesh implemented in the agents as their behavior for simulation. For cartographic visualization, we extracted the shapefile from the sample regions using a GIS. We integrated this shapefile into the multi-agent system were an implementation of the resulting model has been made using the software REPAST SYMPHONY. The observation shows that the consideration of spatiotemporal dynamics in an SIR epidemiological model presents a better reality than the traditional SIR.

The future works will focus on the experimentation in a live situation in order to release the accuracy of the substantial contribution, the improvement of the discretization on any meshing which does not relate to the center of gravity.

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6 Annex





Figure. 9 a. Zone 1 without Diffusion



Figure. 9 b. Zone 1 with Diffusion



Figure. 10 a. Zone 2 without Diffusion



Figure. 10 b. Zone 2 with Diffusion









Figure. 12 a. Zone 4 without Diffusion

