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Research Article

Modelling the spread of covid-19 in the capital of Brazil using numerical solution and cellular automata

André Luís Brasil Cavalcante [a,*], Lucas Parreira de Faria Borges [b], Moisés Antônio da Costa Lemos [c], Márcio Muniz de Farias [d], Hervaldo Sampaio Carvalho [e]

[a] Department of Civil and Environmental Engineering, University of Brasília, Brasília, DF, 70910-900, Brazil
[b] Department of Civil and Environmental Engineering, University of Brasília, Brasília, DF, 70910-900, Brazil
[c] Department of Civil and Environmental Engineering, University of Brasília, Brasília, DF, 70910-900, Brazil
[d] Department of Civil and Environmental Engineering, University of Brasília, Brasília, DF, 70910-900, Brazil
[e] University Hospital and Medical School, University of Brasília, Brasília, DF, 70910-900, Brazil

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ABSTRACT

The novel coronavirus disease 2019 (COVID-19) still challenges researchers due to its spread and deaths. Hence, the classical epidemic SIR and SEIRD models inspired by the epidemic's outbreak are widely used to predict the evolution of the disease. In addition to classical approaches, describing complex phenomena through Cellular Automata (CA) is a highly effective way to understand the iterations on a populated system. The present research analyzed the usage of CA to generate an epidemic-computational model from a micro perspective based on parameters obtained through a statistical fit from a macro perspective. After validating SIR and SEIRD models with the government official data for Brasilia, Brazil, the authors applied the obtained parameters to the Cellular Automata model. The CA model simulated the spread of the virus from infected to uninfected people in a restrained environment (i.e., a supermarket) under several varied conditions applying an approach never adopted before. The manner of applying CA in this research proved to represent an essential tool in predicting the spread of the coronavirus in confined spaces with random movements of people. The CA numerical open-source presented has the purpose of clarifying how the spread occurs not only as a mathematical curve but in an organic way. The numerical simulations from the CA model allowed the authors to conclude that markets and stores are relevant places where might be infections. Thus, every local store and the market owner should reason about the aspects that could avoid the spread of the disease, coming up with efficient solutions. Each environment has specific features that only those who know them are the ones capable of managing.

1. Introduction

The coronavirus (COVID-19) epidemic generates significant social, economic, and health impacts, highlighting the importance of real-time analysis (Tan and Chen, 2020). Continuous models, usually described in ordinary nonlinear differential equations, have formed a significant part of the traditional mathematical epidemiology literature (Vargas-De-León, 2011). Among these models, the predictive model of epidemic phenomena called SIR (Susceptible-Infective-Recovered), and SEIR (Susceptible-Exposed-Infective-Recovered) are frequently used to investigate infection data and epidemic outbreak. These models represent one of the most adopted mathematical models to predict different contagion situations. However, sufficient data need to be available. Then these models can be applied to choose the best restriction and lockdown measures and other restrictive measures in different sectors in the society.

The basis of the SEIR model is a series of dynamic ordinary differential equations that consider the population subjected to contagion and the trend over time of individuals who recover after infection (Godio et al., 2020). The SEIRD model (a version of SEIR) includes death in modeling, and epidemiologic studies use similar models (Korolev, 2020; Lin et al., 2020; Wang et al., 2020). The SEIRD model considers five groups of people: susceptible (S), exposed (E), infectious (I), recovered (R), and dead (D). As a result, the SEIRD model should reflect the

* Corresponding author.
E-mail addresses: abrasil@unb.br (A.L.B. Cavalcante), lucaspdfborges@gmail.com (L.P.F. Borges), moisesaclemos@gmail.com (M.A.C. Lemos), muniz@unb.br (M.M. Farias), carvalho@unb.br (H.S. Carvalho).

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epidemic's progression more accurately than a more conventional SIRD model that does not include an incubation period.

Manners to address and understand the complexity in nature are of great interest to the scientific community. Moreover, as the amount of available computing power grew during the past three decades, the study of dynamical systems has intensified considerably (Ozelim et al., 2016). The Cellular Automata (CA) approach is a numerical method that models time-based and phenomena-based logical components and discrete nature. Describing complex phenomena using cellular automata (CAs) has shown to be a promising approach in pure and applied sciences (Ozelim et al., 2012). The rules of a Cellular Automata case are usually simple, i.e., have basic rules describing the behavior of the cells. The abundance of cells and distinct boundary and initial conditions can generate complex or unexpected results. CA has been studied for a reasonable time (Von Neumann and Morgenstern, 1945; Conway, 1978) and has been extensively explored by modern scientists (Wolfram, 2002; Zubeldia et al., 2016; Ozelim et al., 2018; Wolfram, 2018).

In this research, the data of COVID-19 from the Federal District, Brazil, was used to validate the SIR and SEIRD model results. The collected epidemic data from the Ministry of Health of Brazil (Brazil, 2020a) and the Federal District Secretary of Health (Brazil, 2020b) from February 23th to November 2th, 2020, studied the approximation of the actual and simulated data. After fitting the parameters, the authors simulated the cellular automata for various scenarios of the spread of COVID-19 in a supermarket.

2. Model description

2.1. SIR Model

Kermack and McKendrick (1975) created the susceptible (S) - infected (I) - recovered (R) model, which describes the dissemination of a particular communicable disease in a susceptible population of size *N*. The spreading of the virus (COVID-19) occurs when infected people transmit the illness to susceptible individuals. The transmissible period starts before the symptoms appear and extends throughout the whole course of the disease until the patient's recovery. R is the compartment used for the population infected and then removed from the disease state, either due to immunization or to death. Those in this category are not able to be infected again or transmit the infection to others.

The SIR (Susceptible, Infected, Recovered) model has the following variables: *S(t)* is the susceptible population; *I(t)* is the population who get laboratory positive confirmation and with infectious capacity; *R(t)* is the recovery cases; $N = S + I + R$ is the total population; β is the infection ratio; λ is the coefficient used in the cure rate;

The following ODE system describes the mentioned variables:

$$\frac{dS(t)}{dt} = -\beta S(t)\frac{I(t)}{N} \tag{1}$$

$$\frac{dI(t)}{dt} = \beta S(t)\frac{I(t)}{N} - \lambda I(t) \tag{2}$$

$$\frac{dR(t)}{dt} = \lambda I(t) \tag{3}$$

The model's initial values are S_0 (t = 0), I_0 (t = 0) and R_0 (t = 0). These are the number of people in the susceptible, infected, and recovered categories at a time equal to zero.

2.2. SEIRD Model

The SEIRD (Susceptible, Exposed, Infected, Recovered, Death) model has the following variables: *S(t)* is the susceptible population; *E(t)* is the population exposed to the virus but not infected in the latent period; *I(t)* is the population with positive laboratory confirmation and with infectious capacity; *R(t)* is the recovered cases; *D(t)* is the death number; $N = S + E + I + R + D$ is the total population; γ^{-1} is the average latent time; κ is the coefficient used in the mortality rate.

The following ODE system describes the mentioned variables:

$$\frac{dS(t)}{dt} = -\beta S(t)\frac{I(t)}{N - D(t)} \tag{4}$$

$$\frac{dE(t)}{dt} = -\gamma E(t) + \beta S(t)\frac{I(t)}{N - D(t)} \tag{5}$$

$$\frac{dI(t)}{dt} = \gamma E(t) - \kappa I(t) - \lambda I(t) \tag{6}$$

$$\frac{dR(t)}{dt} = \lambda I(t) \tag{7}$$

$$\frac{dD(t)}{dt} = \kappa I(t) \tag{8}$$

The model's initial values are S_0 (t = 0), E_0 (t = 0), I_0 (t = 0), R_0 (t = 0), D_0(t = 0). These are the number of people in the susceptible, infected, recovered, and death categories at time equal zero.

2.3. Cellular Automata

Cellular Automata represents entities within a discrete space that have determined rules of behavior. These cells, contained in a mesh and having a set of behavioral rules, can interact with each other and affect their states over time. This numerical method is compatible with understanding disease contamination in a controlled environment in its precise nature. While using the Cellular Automata approach, the intention is to maintain a local perspective of how contamination works in a small time frame and limited space. On the other hand, the analytical models have a global approach, both in population size and time, showing the population passing through the disease cycles. Hence, the Cellular Automata simulation is not a replication of the global perspective, but rather it focuses on the analytical model, with a space and time glimpse of a general and broader context.

The particular Cellular Automata Model applied in this study represents a discrete model that intends to mimic a pseudorandom pattern of people's movement within a supermarket. The description of the model is through conditional statements with both deterministic and stochastic parameters. The goal of the Cellular Automata model is to obtain a micro perspective on contamination. It will be considered only two possible states for the people (P_{state}) in the supermarket: those who are susceptible (0) and those who are infected (1). Note that the infected ones here do not show any symptoms but are still capable of contaminating others. This assumption can be reasonably required because most rules do not allow symptomatic people to enter constrained environments such as supermarkets.

Moreover, there is one parameter to be adjusted in the simulation, which is β_{CA}. The β_{CA} parameter is the probability of an infected human transmitting the virus to a susceptible person while they are neighbors. Each iteration and every person generate a specific arbitrary number called the person's chance (P_C). All chances vary from 0 to 1. Suppose a susceptible person gets in contact with infected persons. In that case, the sum of the infected neighbors times β_{CA} should be greater than the person's possibility to be infected. Mathematically the model can be described as:

$$P_{state} = \left[\frac{N_I.\beta_{CA}}{P_C}\right] \tag{9}$$

where P_{state} is the person's state (0 for susceptible and 1 for infected); N_I is the number of infected neighbors a person has; β_{CA} is the numeric parameter subjected to calibration, and P_C is the person's chance. Note that Eq. 9 is valid only for those who are still susceptible and uninfected. Those who are infected do not change over the simulated period.

To better understand how the Cellular Automata rules work, the following images illustrate the proposed model. First, Fig. 1.a shows an uninfected person represented by a green cell in a mesh. The model understands that the person's state cannot change if it has no interaction with the environment (i.e., people) around it. Also, suppose it is the case that the environment only includes healthy people (Fig. 1.b). In that case, there are no possible infections.

Moreover, Fig. 2 shows infected persons represented by yellow cells with a central uninfected person in green. The uninfected person can interact with the close neighbors in a safe configuration (Fig. 2.a) or in a non-safe distance (Fig. 2.b). In Cellular Automata theory, the last configuration is called the Moore neighborhood (Fig. 2.b). Those who are not close enough (Fig. 2.a) cannot infect others, as assumed in the model. Therefore, just the immediate neighbors (Fig. 2.b) are the transmitting vectors.

If an uninfected person has more infected neighbors, then there is a greater chance to get infected and change his/her state. For instance, if a person has two infected neighbors (Fig. 3.b), then the chance to get infected will be two times greater than if there is only one infected neighbor (Fig. 3.a).

As stated before, for each numerical iteration, a variable denominated chance (P) is designated for a person. The chance (P) randomly varies from 0 to 1, changing in every iteration. Also, every infected person has a probability of infection denominated β_{CA}. Hence, if the sum of infected neighbors times the β_{CA} parameter is greater than the chance (P), the healthy person gets infected.

The Cellular Automaton algorithm uses a pseudorandom function to allocate each person in a neighbor spot without conflicting with the nearby people nor the supermarket itself. Each person can move to another cell for every simulated step, which was previously empty and does not conflict with other people's future move. If there is no available spot, the person remains in the same place. The following image (Fig. 4) shows an example of how movement occurs."

One crucial aspect of being incorporated in the modeling is the safe distance factor. Vyklyuk et al. (2021) pointed out that one of the most effective ways to prevent infection is to keep a safe distance consciously. However, results discussing the effects of social distance in modeling the spread of COVID-19 in small places (e.g., supermarkets) in Brazil are not present in the literature or are not well established. Thus, in this paper, the impact of introducing the safe distance was not considered in the CA modeling.

3. Data Source

Using data of the total number of cases, number of deaths, number of recovered, and number of infected people from the public data of the Ministry of Health of Brazil (Brazil, 2020a) and the Federal District Secretary of Health (Brazil, 2020b), the parameters were estimated.

4. Models implementation

4.1. SIR and SEIRD

The authors implemented the coronavirus data and models (SIR and SEIRD) using Wolfram Mathematica 12.1 software. The *ParametricNDSolve* solved Eqs. 1 to 3 (SIR) and Eq.s 4 to 8 (SEIRD). The use of the *NonlinearModelFit* function allowed to obtain the adjustment parameters of the SIR model (I_o, β, and λ) and the SEIRD model (I_o, β, λ, γ, and κ).

4.2. Cellular automata simulation

The Cellular Automata simulation represents a small time frame and limited space representation of the analytical models. It is comparable to a minor part of the infected and susceptible curves from SIR and SEIRD models. Once the analytical models involve more states (those who recovered, died), they also include more parameters. Thus, it is unfeasible to compare every feature. However, the β parameter can be compared to the β_{CA} parameter of the Cellular Automata model.

The β_{CA} parameter in the Cellular Automata model is the probability of an infected person transmitting the virus and infect a susceptible one. The β parameter of the SIR model considers a distinct definition. The average number of contacts per person per time is multiplied by the probability of disease transmission in contact between a susceptible and an infectious subject. Therefore, both parameters are intrinsically related. Correcting the value of β_{CA} and varying the number of people on the simulation, one can achieve the desired β parameter (fitted from the SIR/SIERD model).

With this correlation, the numerical establish scenarios where the analytical model's parameter can be found. Moreover, the practical concern is to understand how the population size variation influences the β parameter. The flowchart of Fig. 5 shows the essential idea of the simulations.

Each complete flow, end to end, result in two practical simulations - one with a smaller population another with a higher population. The first simulation matches the SIR model parameter, and the last allows one to understand the changes in this parameter. At the same time, the β_{CA} is constant while the community size changes from the previous simulation.

The simulated scenarios occur in a supermarket where each mesh cell is a 0.6 m sized square. Each person is a colored cell that can move randomly across the supermarket's white space and its entrance

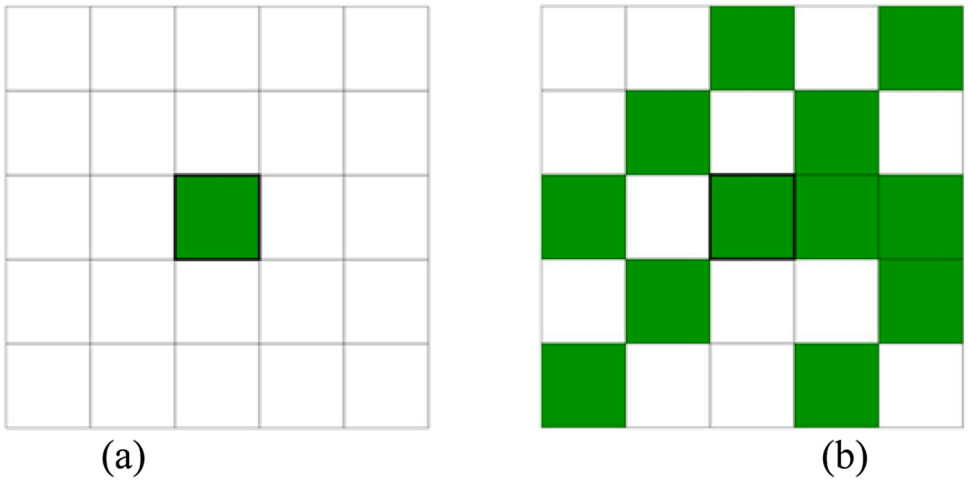

Fig. 1. Uninfected person isolated (a) and surrounded by others uninfected (b).

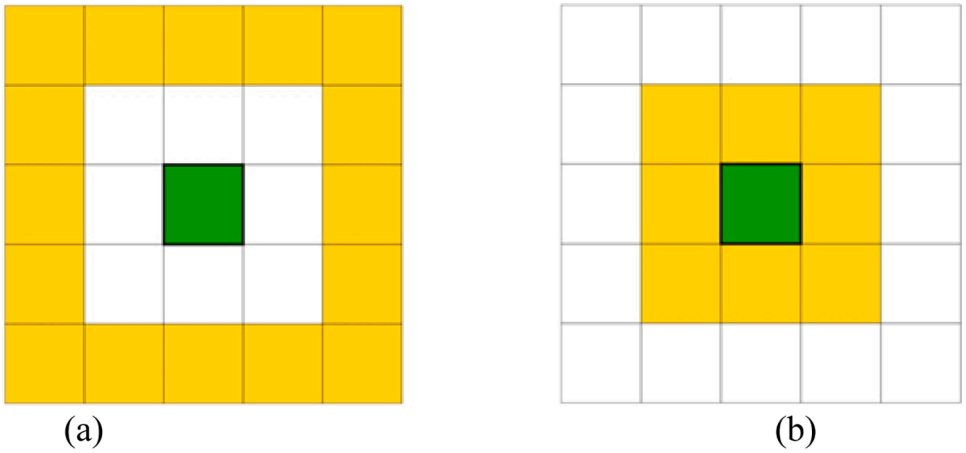

Fig. 2. An uninfected person surrounded by infected persons (a) and unsafe (b) conditions.

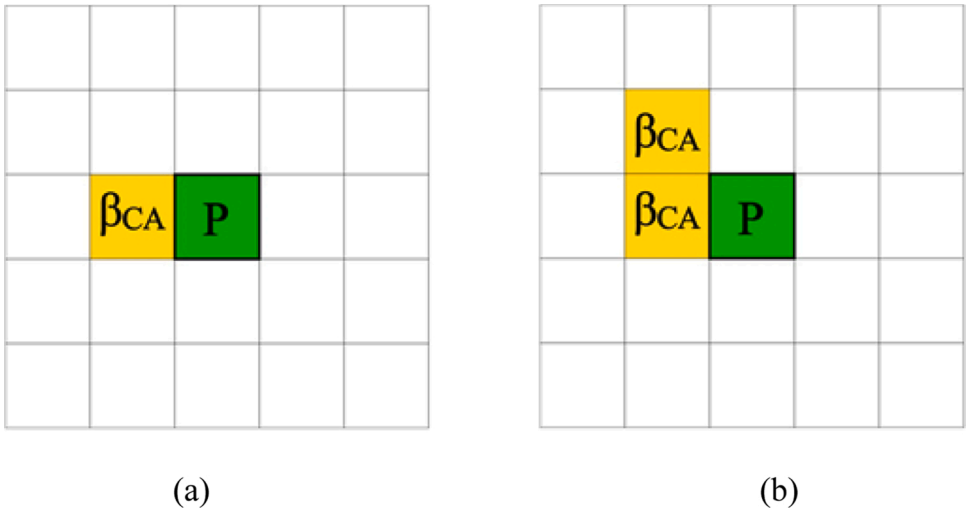

Fig. 3. An uninfected person surrounded by one (a) and two (b) infected neighbors.

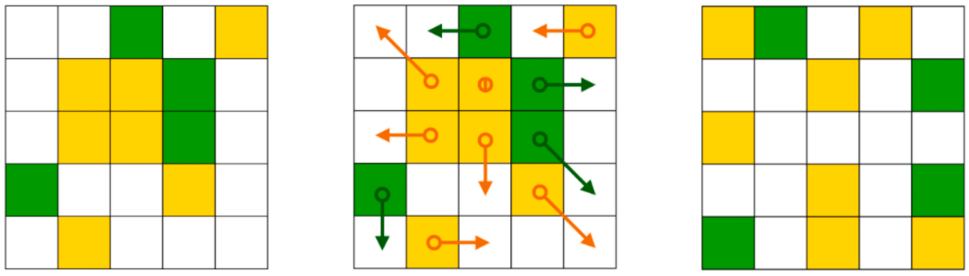

Fig. 4. Cellular Automaton algorithm illustration.

proximities. The yellow cells correspond to the infected (1), while green cells are susceptible (0). The gray cells represent the supermarket structure and constrain the movement of the population. The total period of the simulation is 180 min. The time step is 1 min, which is when every interaction between people and movement occurs.

5. Results and discussion

5.1. Application of SIR and SIERD models

The adjustment of the data made available from COVID-19 in the Federal District for the SIR and SIERD models considered 02/23/2020 as t = 0. The adjusted data refer to 11/2/2020 (t = 253 days).

Figs. 6,7 and 8, show the model fitting for data from COVID-19 in Brasilia. The solid lines are the simulated values using SIR and SEIRD models, and the points are the data collected. Table 1 shows the adjusted parameters. Both models had their parameters (those that are similar) reasonably the same.

The Akaike information criterion (AIC) (Akaike, 1974) made a comparison between both models. The AIC is a technique based on the sample fit to estimate a model's likelihood to estimate future values. The quality of the model is the one that has minimum AIC. The SIR model had an AIC of 9177.53, and the SEIRD model had 13.485,9. Thus, the SIR model was better than the SEIRD model. However, the latter is more

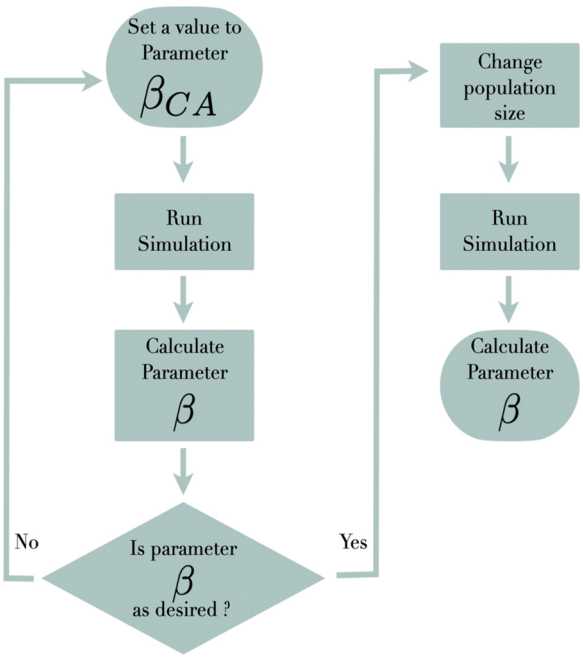

Fig. 5. Methodology of the cellular automata method.

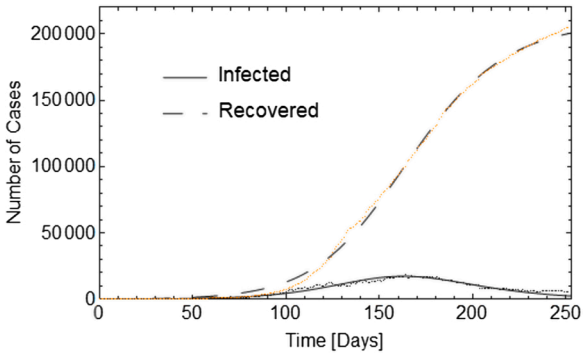

Fig. 6. Fitting of SIR model.

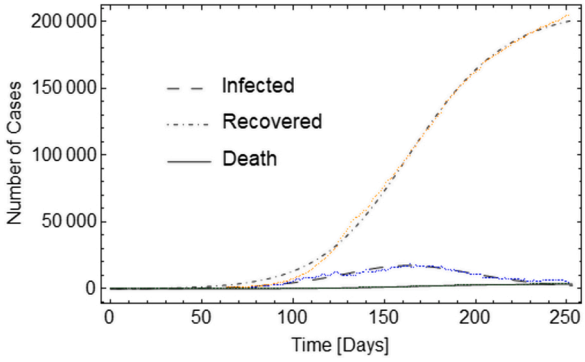

Fig. 7. Fitting of SEIRD model.

crucial to obtain the number of dead people.

5.2. Cellular automata scenarios

The simulation considered four scenarios applying the Cellular Automata model (Table 2). Two simulations correspond to the SIR parameter value (β_{SIR}). The other two do not match the analytical

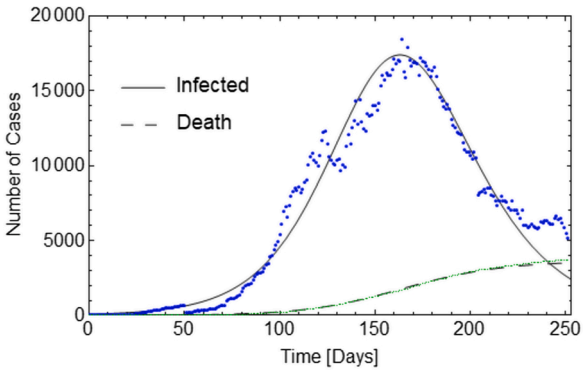

Fig. 8. Fitting of SEIRD model (infectious and death).

Table 1
Parameters estimated by SIR and SEIRD models.

Parameter	SIR	SIERD
β	0.160664	0.164682
λ	0.116857	0.117336
γ^{-1}	–	2.2703
κ	–	0.002044

Table 2
Parameters and initial conditions of the numerical simulations.

Scenario	Parameter		Initial state	
	β_{CA}	β	*Infected*	*Susceptible*
1	0.025	0.16	4	16
2	0.025	0.90	20	80
3	0.005	0.160	20	80
4	0.005	0.016	4	16

parameter but keep the numerical parameter value with changes in the population size. The CA simulations consider the beta model of the SIR model. However, the time of the simulations is too short to consider any recovery of the population ($\lambda \rightarrow 0$), making the SIR model behave as the SI (susceptible and infected) model. Therefore, CA simulations do not consider the recovered people and focusing on the susceptible and infected.

The first and the fourth simulations describe 20 people inside the supermarket, while the second and the third simulations represent 100 people. The difference in size between the populations is 400 %, but the initial proportion of infected and susceptible is the same. The parameters are observed not by a unique simulation but through the average of several simulations and thirty simulations for each parameter. Each simulation has stochastic parameters related to both the movement and the chance of being infected. Thus, it was necessary to run each case several times to find a mean curve.

Fig. 9 shows the supermarket occupation. Not only have people inside it, but also by its entrance, as stated before. Fig. 9.a stands for the case where there are only 20 people, where Fig. 9.b has a total of 100 people.

The simulations of scenarios 1 and 2 compose a pair, described in the flowchart of Fig. 5, and they share the exact parameters of Table 2, respectively. Fig. 10 shows the initial simulation ($t = 0$) for all scenarios. Fig. 11 shows the simulation in the time of 90 min for all scenarios. Fig. 12 shows the simulation for 180 min for all scenarios. Figs. 13 and 14 show the variation of the number of persons infected and susceptible for scenarios 1 and 4 and 2 and 3, respectively.

Scenario 1 describes where the β parameter is equal to 0.16, representing the value obtained on the analytical curves, as seen in Table 2. This simulation takes only 20 people, where four are initially infected

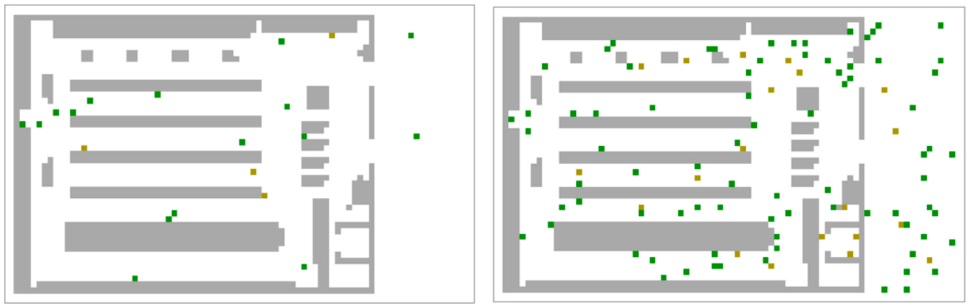

Fig. 9. Sample initial condition for (a) 20 people and (b) 100 people.

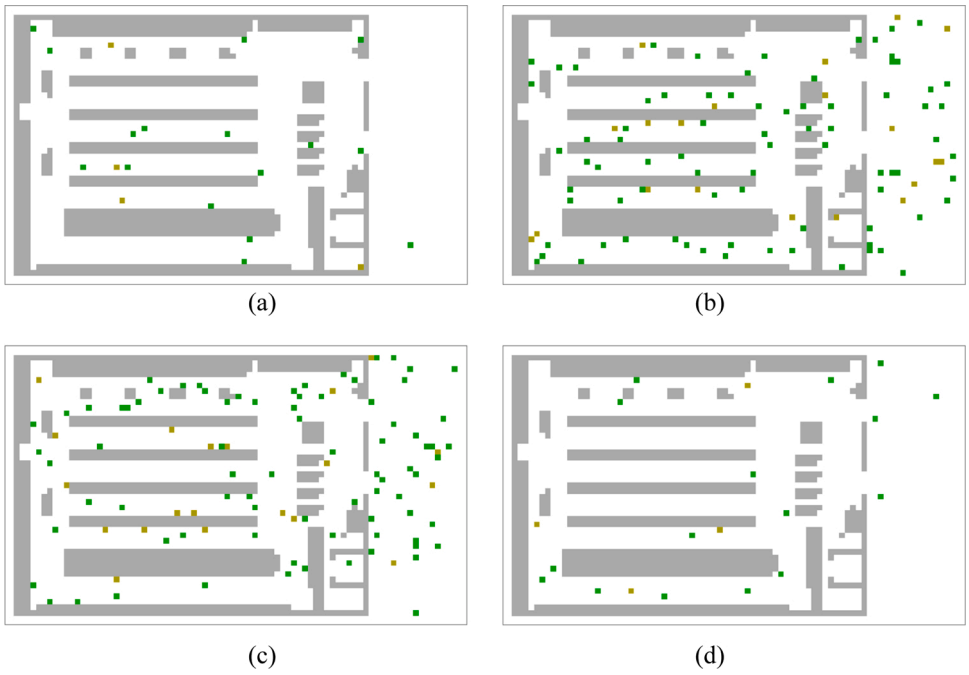

Fig. 10. Initial condition of simulation for (a) scenario 1 (b) scenario 2, (c) scenario 3, (d) scenario 4.

and 16 are susceptible (Fig. 10.a). Conducting 30 simulations and assuming their average, it is possible to represent the mean curve and the distribution for each scenario. Also, one of these 30 simulations represented the evolution of the state through time for each scenario. These particular simulations were randomly chosen and represent every 30 min out of the 180 min simulation. Figs. 11.a and 12 .a show scenario one at 90 min and 180 min, respectively. On the mean curve charts (Figs. 13 and 14), the continuous lines represent the mean curves, while each scattered dot corresponds to a specific time and population size of one out of the 30 simulations

Scenario 2 (Figs. 10.b, 11 .b and 12 .b) has 100 people - 20 infected (yellow) and 80 susceptible (green). In this second simulation, the β_{CA} parameter is kept the same as the first one, which implies a different β parameter, once there is an increase in the population. As expected, the β parameter has significantly increased.

Scenarios 3 and 4 compose a pair, either. Simulation 3 (Figs. 10.c, 11 .c and 12 .c) begins with 100 people - 20 infected and 80 susceptible. This simulation has the same β parameter as the one found in Table 4 from the analytical fit. Similar to the previous cases, one simulation was chosen to be represented by 30 min steps. This specific simulation shares the same parameters as seen in Table 2.

Then, simulation 4 (Figs. 10.d, 11 .d, and 12 .d) keeps the same numerical parameter β_{CA}, but with a smaller population - a total of 20 people with 4 infected and 16 susceptible. This simulation shows how a reduced number of people in a constrained space drops to close to zero infections, even though there are intense movements for three consecutive hours (Fig. 13).

An aspect of being highlighted is that the parameter β_{CA} is linearly inversely proportional to the population simulated. When the population is multiplied by five, to have the same β parameter, the numerical parameter β_{CA} needs to be divided by five.

As it can be interpreted from the charts (Figs. 13 and 14), if the numerical parameter β_{CA} is constant, but the population simulated increases, it results in more infected cases. An increase of the allowed population inside a constrained environment accentuates the curve steepness. The chart results, although they required computational effort, could be qualitatively generated purely by inspection. Hence, all standard policies must be more careful to avoid crowded stores and supermarkets.

Moreover, Fig. 14 shows that if one significantly reduces the number of people inside an environment, the number of infections drops to marginally zero. Markets can be environments of a significant number of infections. Thus, policies should allow stores and supermarkets to open for more extensive periods throughout the day and regulate the number of people.

The chart in Fig. 15 is a numerical curve based on a tridimensional interpolation of scattered points. The curve demonstrates how the number of newly infected people happens after a 180 min interaction in

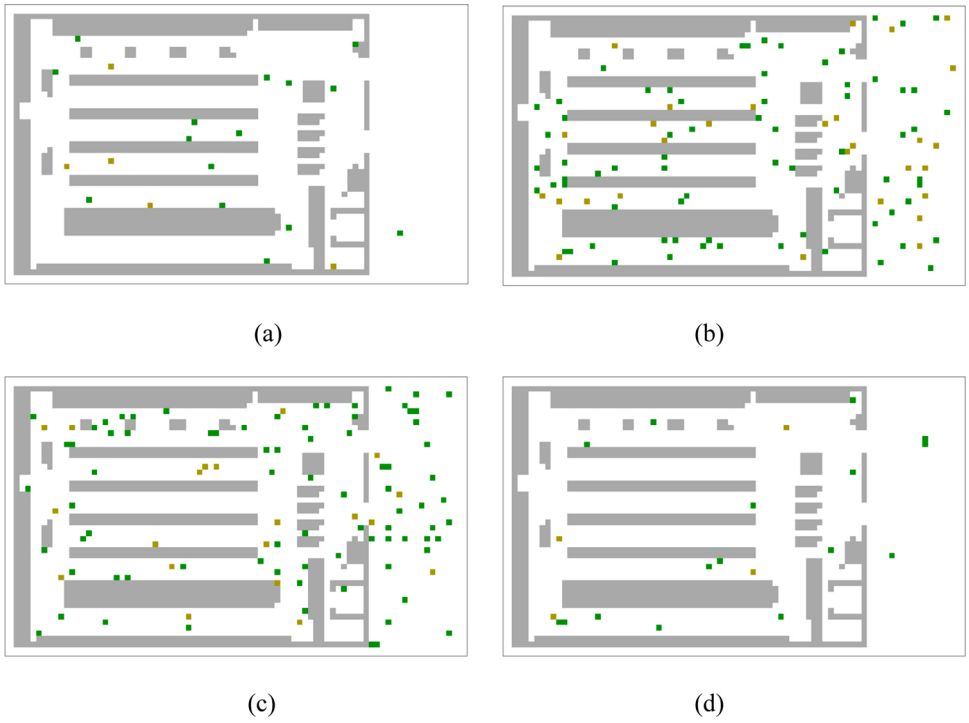

Fig. 11. 90 min of simulation (a) scenario 1 (b) scenario 2, (c) scenario 3, (d) scenario 4.

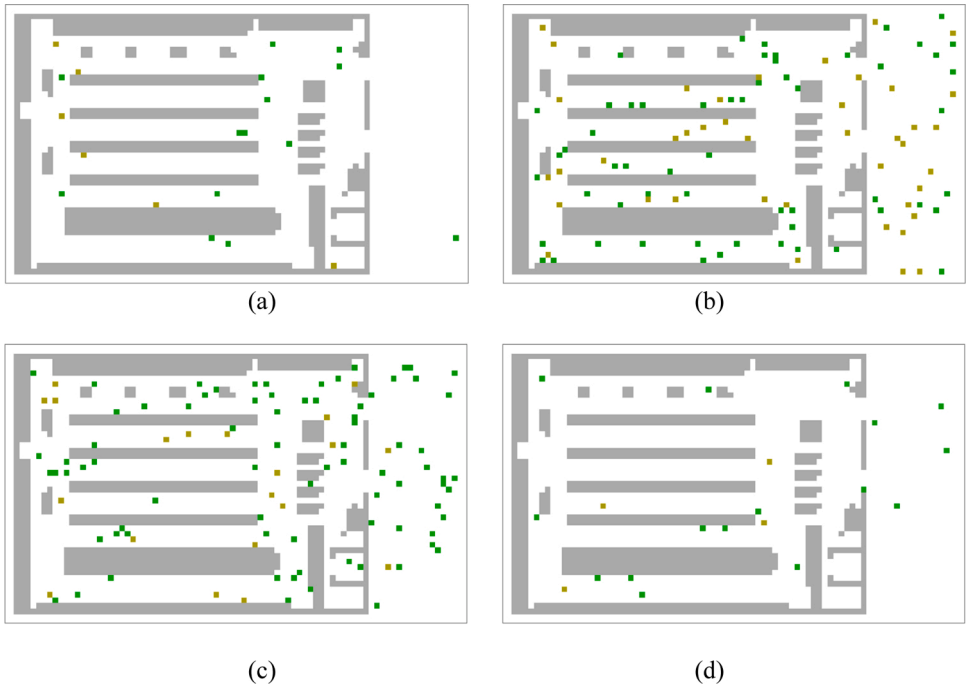

Fig. 12. 180 min of the simulation of (a) scenario 1 (b) scenario 2, (c) scenario 3, (d) scenario 4.

the supermarket, for different infection rates and the total number of people. This curve has a fixed initial rate of 20 % of infected to 80 % of susceptible. As one can notice, the curve becomes steeper when both the β parameter and the number of people are higher than 0.015 and 60, respectively.

Fig. 16 shows the simulation for an initial simulation with 80 susceptible people and 20 infected people. The simulation refers to the transient variation in the number of infected people for different values of β_{CA}. In the case of a higher β_{CA} value, the greater is the spread of the disease. Thus, the knowledge of this parameter is of great importance so that the spread of the COVID-19 in small spaces is coherently known using the CA theory.

Schimit (2020) simulated through a Probabilistic Cellular Automata the evolution of COVID-19 in Brazil. The mathematical model presented describes the disease in-depth, with eight possible states with 15 parameters to be adjusted. The purpose of this probabilistic model was to describe the spread of the disease from a macro perspective, considering its cycle and all possible situations, along with the analysis of lockdown

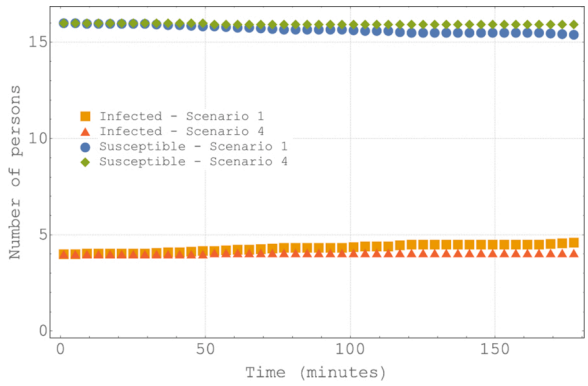

Fig. 13. Simulation curve of scenarios 1 and 4.

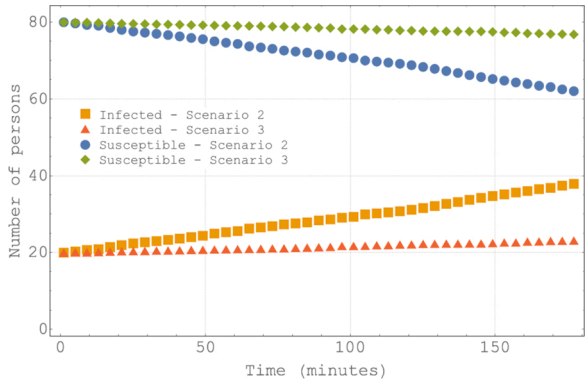

Fig. 14. Simulation curve of scenarios 2 and 3.

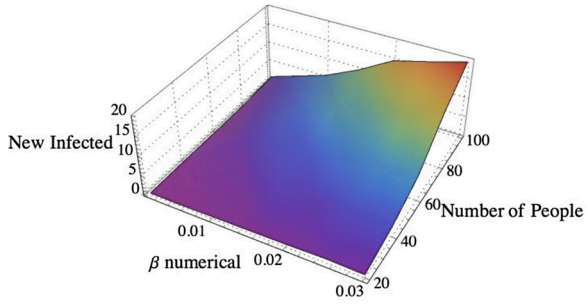

Fig. 15. Number of newly infected people after a 180 min interaction for different β_{CA}.

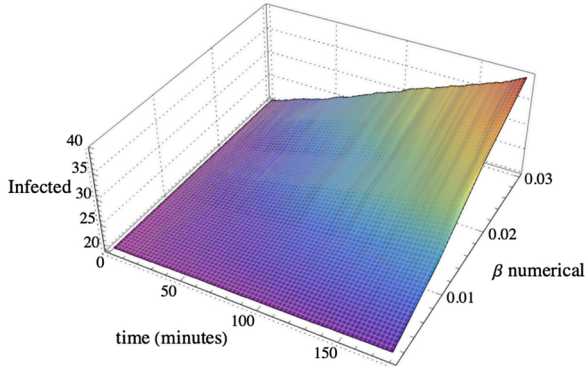

Fig. 16. Transient variation in the number of infected people for different values of β_{CA}.

and healthcare conditions. Although the discrete model presented in this study is also a Probabilistic Cellular Automata, there are two main differences from what the author shows. First, the current intent is to simulation a micro perspective - the spread of the novel coronavirus in a confined space within a few hours. Thus, the model does not require as many parameters or states because only susceptible and asymptomatic are present in this space. Second, the confined space where the cellular automata elements are placed does have a geometric meaning - the restrictions of movements represent a market. Schimit (2020) does not mention any unique geometry of the simulated mesh or discuss elements' movement.

6. Conclusion

The traditional mathematical epidemiology theories are appropriate tools to understand and predict the time evolution of disease outbreaks. These tools are valuable to guide countries and cities in decision-making.

In this research, the classic SIR and SEIRD models helped predict and obtain parameters and the number of susceptible, infected, and deceased people in Federal District, Brazil. The simulations were supplemented by recorded data from the Ministry of Health of Brazil and the Federal District Secretary of Health. The fitted simulation indicated good agreement with the data, and the obtained parameters allowed good results.

After predicting the SIR and SEIRD parameters, the cellular automaton simulated a supermarket case using the parameters obtained in the models. Thus, the lockdown policy used in many cities across Brazil, which closed retail and department stores, has to be more careful about not redirecting people to supermarkets. The present simulations lead to the perception that markets and stores are relevant places with infections. Thus, every local store and the market owner should reason about the aspects that could avoid the spread of the disease, coming up with their solutions. Another practice limiting supermarkets' opening and closing times, which may increase people's concentration inside constrained environments, is not recommended.

Author statements

Please find below the data availability statement of the paper entitled "Modelling the spread of covid-19 in the capital of Brazil using numerical solution and cellular automata" coauthored by Lucas Parreira de Faria Borges, Moisés Antônio da Costa Lemos, Márcio Muniz de Farias and Hervaldo Sampaio Carvalho from University of Brasília.

André Luís Brasil Cavalcante: Supervision, Project administration, Funding acquisition, Software, Writing- Reviewing and Editing

Lucas Parreira de Faria Borges: Conceptualization, Methodology, Software, Writing- Original draft preparation, Formal analysis

Moisés Antônio da Costa Lemos: Conceptualization, Methodology, Software, Writing- Original draft preparation, Validation

Márcio Muniz de Farias: Writing- Reviewing and Editing, Funding acquisition

Hervaldo Sampaio Carvalho: Writing- Reviewing and Editing, Funding acquisition

Data availability statement

All data, models or code that support the findings of this study are available from the corresponding author upon reasonable request.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary material related to this article can be found, in the online version, at doi:https://doi.org/10.1016/j.compbiolchem.2021.107554.

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