Toward an Agent-Based and Equation-Based Coupling Framework

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Abstract. The ecology modeling generally opposes two class of models, equations based models and multi-agents based models. Mathematical models allow predicting the long-term dynamics of the studied systems. However, the variability between individuals is difficult to represent, what makes these more suitable models for large and homogeneous populations. Multi-agent models allow representing the attributes and behavior of each individual and therefore provide a greater level of detail. In return, these systems are more difficult to analyze. These approaches have often been compared, but rarely used simultaneously. We propose a hybrid approach to couple equations models and agent-based models, as well as its implementation on the modeling platform Gama [7]. We focus on the representation of a classical theoretical epidemiological model (SIR model) and we illustrate the construction of a class of models based on it.

Keywords: Equation-based model · Agent-based model · Coupling framework · Simulation platform · Epidemiology

1 Introduction

Mathematical modeling and agent-based modeling are two kind of modeling often used for describing dynamical systems [4]. Equation Based Models (EBM) are present in many domains, such as physical, chemical, biological, economical systems [4,5]. Agent-Based Models (ABM) appeared with the development of computer science, which allowed describing large complex systems [15]. In particular, both kind of modeling are used in epidemiology. The well known SIR model [2,9] is the first epidemiology model that has been developed in 1927. It is a compartment level that allows describing the dynamics of an epidemic at the population level according to very simple assumptions. SIR models and their derivative (spatial mathematical models using partial differential equations) were

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extensively used for many diseases and real case studies. ABM models were later developed in order to introduce a description of processes at a finer level [10]. They describe the propagation of epidemics by representing the processes at the individual level.

Those two kinds of modeling paradigms are often used to represent the same systems, with different benefits and drawbacks. As a global approach, EBM models require very little resources and allow performing a complete mathematical analysis of the system (equilibria, stability, asymptotic behavior, etc.). However, heavy preliminary work is need in order to determine how the processes involved in the dynamics can be translated into mathematical equations. Furthermore, representing such processes at the global level leads to a loss of information corresponding to individual variability. Contrarily, ABM use a local approach and allow a detailed description of processes occurring at the individual level. Such description is more intuitive and better represents variability. On the other hand, ABM require a high amount of resource depending on the number of agents that are represented and a high amount of data depending on the level of details described, while EBM usually do not. Therefore, ABM are more difficult to analyze and have more risks of over fitting. The main objective of our work is to propose a coupling methodology of equation-based models and multi-agent-based models. With this method, modeler can take advantage of both approaches, switching from individual level to global level when needed. This work also offer a programmable environment for both formalisms.

This paper consists of six parts, the first being this introduction. The second part introduces related works about coupling the two modelling approaches. In the third part, we present a methodology for coupling the agent-based and the equation-based approaches. In the fourth part, we present an implementation of our method into the simulation platform GAMA. The fifth part is dedicated to experimental results, and the sixth part to discussion and ongoing work.

2 Related Work

In this part, we present the current state of the art of coupling two modeling approaches: Agent-Based Modeling and Equation-Based Modeling. Although these two approaches aim at a common objective, they are distinct by their modeling formalism. The necessity of coupling and comparing the two approaches has been raised in several research studies. They use a common methodology: exploration is always done by implementing an agent-base model beside an equation-based without the support of an agent-based modeling framework neither an equation-based framework.

In [17], the authors study the difference between agent-based modeling and equation-based modeling in a industrial supply network project in which network's domain supply are modeled with both agents and equations. They also summarize the resemblance and variety of two approaches with a suggestion to use one or another. Their study is part of the DASCh project (Dynamical Analysis of Supply Chains). DASCh includes three species of agents: Company agents, PPIC agents and Shipping agents. It also integrates a fixed set of ordinary differential equations (ODE).

Coupling and comparing agent-based and equation-based is also found in [14] where Rahmandad et al. examine in contrast the dynamic of well-know SEIR model which describe the common and important context of the spread of contagious disease. They compare and validate an ABM and EBM for epidemiological disease-spread models, as well as [16] who use an ABM and EBM of the 1918 Spanish flu. In their publication, they propose a model validation framework of choosing ABM or EBM.

Nguyen in [12] propose to use only one appropriate modeling formalism instead of two approaches, and infer an EBM from an ABM SIR model by exploring the deducible parameters like number of individual in population, rates of interactions base on dimension of environment, ... They have done a study with the measure based on disk graph theories [11] to link ABM with EBM dynamical systems applied to theoretical population ecology.

Another coupling approach is proposed in [1,13] or [3]. In the simulation of emergency evacuation of pedestrians in case of a tsunami in Nhatrang City, Vietnam, people move along the road networks as agents. The agent based model of individuals movements are replaced by equation models for the roads with higher traffic. This transformation give the model an addition of time and resource for such evacuation model which usually take into account huge populations (Fig. 1).

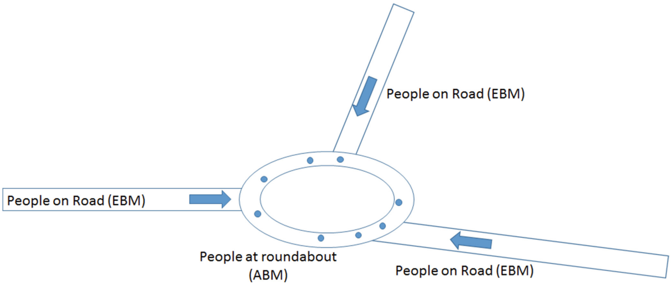


Fig. 1. Coupling approach example: people moving on the road are represented in the form of equation, and in form agents at the crossroads

All these approaches provide mechanisms that allow interaction between several models but they still have the following disadvantages:

- In general, these approaches are not generic and are difficult to be re-implemented in different domains and contexts.
- There are no consideration of the differences in spatial and temporal scales.
- Their are no framework that support coupling of heterogeneous models between equation-based modeling and agent-based modeling paradigm.

3 Coupling Between Equation-Based Model (EBM) and Agent-Based Model (ABM)

3.1 Equation-Based Model

The equation-based models [4] predict the long-term dynamics of the studied systems. They use mathematical formalism based on Ordinary Differential Equations or Partial Differential Equations. The modelling approach is generally driven by the principle of parsimony (or *Occam's razor*), which means that the model should be kept as simple as possible, with as few parameters as possible. Although, if a stochastic approach is possible, a deterministic approach is preferable when possible. In addition, processes are considered at a global scale (e.g. in ecology: at the population level instead of the individual level), assuming that the processes that govern the system at such a scale can be determined (often using mean field approximation). For example, the demographic dynamics of a population can be described at the global level using a parameter call *population growth rate*, which can be derivated from the mean of offsprings per individual per time unit. Due to such approximations, the variability between individuals is difficult to represent, making these models more suitable for large and homogeneous populations. Mathematics often provide useful analytical tools to find the properties of ODE models, such as equilibria and asymptotic dynamics. The evolution of the system can be determined from mathematical proofs, which are more robust than just simulations. For those reasons, such models can be easily analysed and are useful for making predictions. On the contrary, translating the studied processes into equations requires a good knowledge of similar physics or mathematical models. Processes also have to be sufficiently smooth in order to fit their mathematical description. As a summary, such models require a large amount of work upstreams, but they offer conceptually good possibilities of analysis downstreams (the technical issues that could be encountered in mathematical proofs is not discussed here).

EBMs have been wildly used for epidemiology modeling. A pragmatic reason is that mathematical analysis methods were the only available methods, as computers and EBM were not available to Kermack and McKendrick in 1927. However, there are many conceptual reasons why EBM are a reasonable choice for modeling epidemics. Firstly, epidemics arise in large populations, and the transmission and remission rates variability among individuals can be easily represented according to familiar distribution laws, making such processes easy to describe at the population level using mean field approximations. Secondly, the analysis of the equations provide useful prediction tools for epidemiology: one can determine conditions on the parameters for which the epidemics will arise or not. For example, the basic reproduction number R_0 can be computed with the parameters of the model, based generally on transmission and remission rates. Values greater than one mean that an epidemics outbreak will occur, such an event can be then predicted without simulations.

3.2 Agent-Based Model

Agent-based models [6] are used to represent the attributes and behavior at the individual level, and therefore to provide a greater level of detail. They can describe strong individual variability, not only for the attributes of the individuals of a same population, but also for their behavior. They are often associated to small time scales, which correspond to the individual processes time scales. In return, these systems may be more difficult to analyze and prediction almost rely on simulations (apart from some ABMs which are actually probabilistic mathematical models that can be analysed with mathematical tools). Because of the large number of parameters, it can be difficult to test the model sensitivity to one of them. A large amount of analysis, dependent on simulations and on the assumed prior distribution of parameters has to be performed in order to provide synthetic results. ABM use a specific language to describe in detail the aspects of agents: perception, action, belief, knowledge, goals, motivation, intention, reflexion, etc. Processes can be written as algorithms, offering more freedom to the modeler, as complex decision structures can be used (e.g. if the behaviour of individuals depends on some condition, an *if-then-else* construct can be used). The ABM approach also proposes a more intuitive way to build the model: processes can be represented as close to the perception of the modeler. As a summary, such approach proposes an easy and intuitive work upstreams, but requires a large amount of work downstream to provide relevant results. In addition, the large number of parameters combined with the often large size of population considered means that such a model may need a very important amount of resources to run simulations.

Interest of epidemiologists in ABMs relies on the ability to give a detailed description of the network of transmission, and such models have been developed alongside graph theory. Such models are useful to represent singular events (one infected individual entering a large susceptible population) and the stochasticity associated to such events. Such models are used to represent the worldwide propagation of infection due to air travel. Depending on the disease, a detailed behavior of the infection vector can be given.

3.3 Coupling EBM and ABM

These approaches have often been compared but rarely used simultaneously.

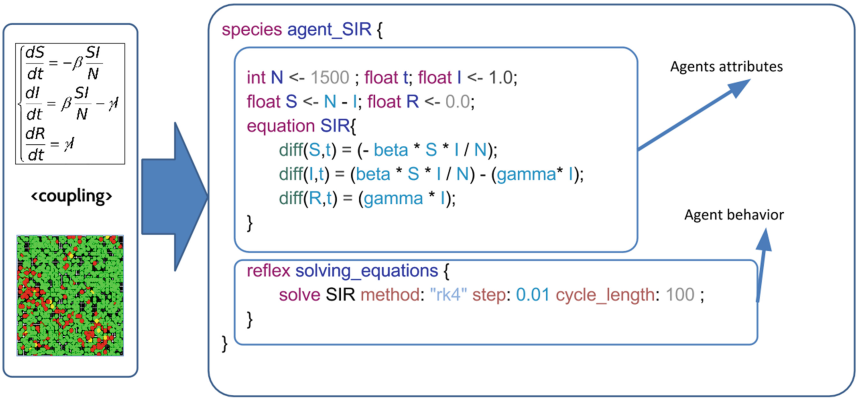
Coupling problems. In this part, we introduce the existing problems in many researches which have been done to couple the models of complex system in multi-discipline:

Different formalism of modeling: Coupling models often takes place when modelling is carried out with more and more models from many different domains, such that each one comes with a particular modeling formalism. Thus, modeler is led to the problem of diversifying the formalism of coupling models. In this research, ABM is based on agent formalism and the EBM is based on the algebric equation paradigm.

Spatial - temporal scale: While coupling ABM and EBM models, modeler usually encounters with the need to change the spatial and temporal level of an object or of models components, to have benefit with diverse representation from one model to another. Each model has its own scales and needs to take into account entities at different spatial and temporal scales. For example, models in epidemiology may need to represent explicitly entities that belong to a hierarchy of containers, like molecules, cells and tissues. Their spatial scale has multiple levels of observations: ward, commune, district, city, region, etc., as well as multiple temporal levels of observation: days, weeks, months, quarters, years, couple of years...

Explicit description of the coupling: There are no ways to support the explicitly description of the coupling between ABM and EBM. The problem pose is to describe how the sub-model will interact each other. Most of all research proposed coupling research implicitly implement the integration of models. They have been done on the coupling between ABM and EBM, is based on the exchange value during or after simulations. In that case, the composing is fixed and could not be changed easily and dynamically with an explicit modeling language. It leaves aside the semantic problem to describe the dynamic of coupling and composition.

Propose methodology. In the act of our research domain which is present in [8] to propose a coupling framework that support the modeling and simulation of complex systems, we propose in that scope an approach to compose the two modeling types (ABM and EBM) in one modeling environment. This methodology will facilitate the comparison between the two types of models through the combination and simultaneous use (Fig. 2).



```
species agent_SIR {
    int N <- 1500 ; float t; float I <- 1.0;
    float S <- N - I; float R <- 0.0;
    equation SIR{
        diff(S,t) = (- beta * S * I / N);
        diff(I,t) = (beta * S * I / N) - (gamma* I);
        diff(R,t) = (gamma * I);
    }
    reflex solving_equations {
        solve SIR method: "rk4" step: 0.01 cycle_length: 100 ;
    }
}
```

Fig. 2. Coupling between ABM and EBM: equations are integrated into agents

3.4 Model “Switch”

We illustrate our coupling methodology by implementing a hybrid model, called Switch, combining equations and agents on the modeling platform Gama. We build a class of SIR model based in both ABM and EBM (Fig. 3), in which people are represented by agents when the density is low, and by equations if the density is higher, a tilting mechanism for moving from an approach to another.

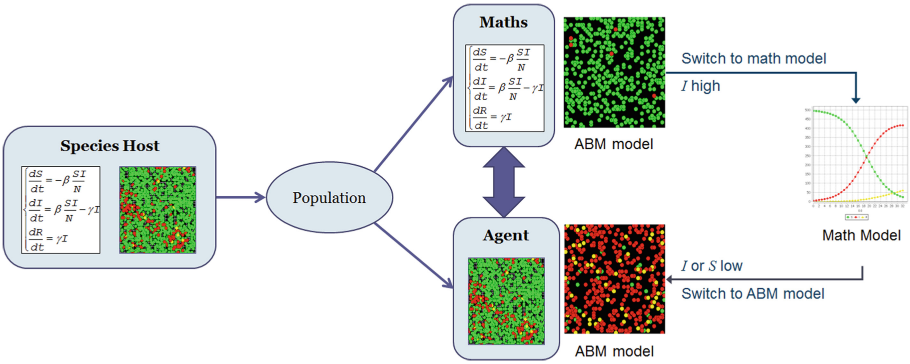


Fig. 3. Representation the dynamic of “Switch” model

Both models are based on the same assumptions. They involve two processes: contamination and recovery. The ABM model also adds spatial interactions and dispersal. The mathematical model is indeed a mean field approximation of the ABM and represents the dynamics at the global scale, while ABM shows the dynamics at local scale. The contamination and recovery processes happen frequently with a “uniform distribution” over time.

- Assumption (i) implies that processes can be represented at a continuous time;
- Assumption (ii) allows to replace probabilities of processes occurrences by expectancies; finally assumption (iii) allows to consider that all individual have the same number of neighbors.
- Assumption (iii) populations are considered to be at sufficiently high density; populations are considered as homogeneous for spatial distribution of individuals, as well as for the distribution of each type of individuals (S, I and R).

Considering that assumption (i) holds is rather natural, as processes occur along constant time steps. Epidemiological models usually assume that population densities are high, thus condition for assumption (ii) seems to be naturally fulfilled. However, in a large population, the density of infected (or even susceptible) individuals may be very low. Indeed, a usual condition for such kind of model is the introduction of a small group of infected inside a disease free population. Mathematical model are deterministic and ignore the variability due to stochasticity which alter the dynamics: if one infected individual is introduced in the population, if basic reproduction rate R0 > 1, and epidemic outbreak will be predicted by the mathematical model. However, in real cases or for ABM, there is a chance to avoid epidemic outbreak as contamination may not occur thanks to the stochasticity of infection process. Assumption (iii) may not be possible for spatially explicit ABM, as spatial distribution does not remain constant and spatial patterns could appear, like contamination waves. Assumption (iii) makes that the EBM, as mean-field approximation of ABM, is also the "limit" (in the mathematical sense) of the EBM when spatial process tends to spatial homogeneity, which is achieved by letting the neighborhood of an individual tend to cover the whole environment, or by increasing the speed of movement of individuals (well mixed populations).

Comparing both EBM and ABM is exhibiting the differences due to approximations done for the ABM model due to assumptions (ii) and (iii). Assumption (ii) is at the heart of the model switch problematic: EBM should not be used when the conditions for this assumption are not fulfilled. Assumption (iii) also add a challenge to model switching, as corrections have to be made in order to represent into the ABM the effects of spatial structures that have been hidden by the approximation made with this assumption. Furthermore, switching from EBM to ABM introduces an explicit spatial distribution of individuals, for which assumption (iii) doesn't have to be made. The spatial distribution, hidden in the EBM, may have to be generated.

The two models are based on SIR models assumptions. Individuals can be in three different states: susceptible individuals (S): the individual is disease-free and can be contaminated by contact with an infected individual (I). After some time, infected individuals recover from the disease (or die). They are assumed to be in a recovered state (R): they are immune to the disease and do not take part anymore in the infection dynamics. The models involve the following processes:

- infection: transmission of the disease from infected individuals. This depends on the contact rate between susceptible individuals and infected individuals;
- recovery: infected individuals heal and recover from infection;
- movements: individuals are assumed to move within the considered environment. There are two type of movement, one is random walking and other is not random, (Fig. 4).

Hypothesis found in both models:

- Recovery rate: the remission rate is very similar in the agent-based model and the equation-based model. In the ABM, parameter gamma is the probability to recover per time unit. In the EBM model, the parameter gamma is a mean-field approximation, which means that the number of recovered individuals given by the EBM model is exactly the expectancy of the number of recovered individuals given by the ABM model (provided that there is no infection occurring at the same time). Stochasticity of recovery rate appears at low I populations, otherwise both models fit.

- Contact rate: in the present models, contact are defined in a similar way for the mathematical model and the agent-based model. In the agent-based model, two individuals are considered to be "in contact" if they are in each other's vicinity for one time step. In mathematical model, space is not explicitly represented, but the average number of neighbours can be determined. Stochasticity of contact rate appear because of size of neighbourhood (strong variability in number of hosts neighbours) and speed of hosts (low speed means no mixing, neighbourhood proportion of R and I may greatly vary).

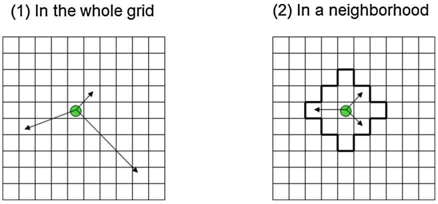


Fig. 4. Two type of deplacement of agent in an environment

We compare this model with existing models and present a method to determine the parameters for transitions between models. In particular, we establish a link between the parameters of the mathematical model, and the representation of contacts and travel agents in a spatial environment.

We are also interested in how to compensate for the loss of information on spatial structures when we move an agent model to a mathematical model. Currently, we save the attributes, especially the location and the status, of all agents and re-assign to agents when they need. We are also interested in how to compensate for the loss of information on spatial structures when we move an agent model to a mathematical model. Currently we have implemented two following method of creation new distribution after the switch from EBM to ABM.

4 An ODE-Integrated Environment

We tackle these problems of differences with our proposition of coupling by integrating these two approaches in a modeling and simulation platform, GAMA [7], in which the equation-based model is declared as an attribute of the agent. It has two famous examples of equation-based modeling which are the Lotka and Volterra [24] modeling of prey-predator dynamics or the Kermack and McKendrick [2] SIR model to represent epidemic dynamics.

We have introduced in GAMA the possibility to describe the dynamics of agents using a differential equation system and to integrate this system at each simulation step. With the enhancement of GAMA modeling language (GAML), modelers have possibility to write equations linking agents attributes and to

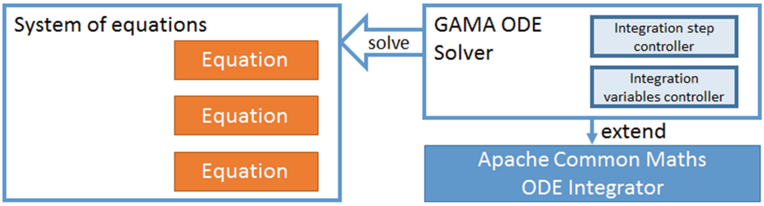


Fig. 5. An ODE solver structure inside a modeling and simulation platform

integrate equation-based system with agent-based system. The GAML syntax permit to write an system of equations of most EBM based on the implementation with Commons Mathematics Library.

To figure out the coupling problem of different temporal scale, we introduce the controller of integration steps and simulation steps beside the two current integration method Runge Kutta 4 and Dormand-Prince 8(5,3). This controller is maintain in the solve statement of GAML and would be call at each simulation step. In the Fig. 5, an equation-based model in form of algebrics is represented into GAML syntax that are called Equation. Set of equations make a System of equations. This type of entity will be integrated by our GAMA ODE (Ordinary Differential Equation) Solver package.

5 Experiments

5.1 Objective, Data and Tools Used

In this part, we do experiment to prove the capabilities of coupling framework that we have proposed to compose the ABM and EBM. The experiments will have three scenarios, each scenario The data used in the "Switch" model is bring in the real data of SIR model. The epidemiology's parameters are the spead of the flu and measles.

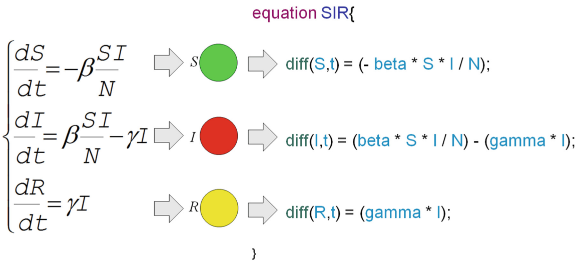
5.2 Represent Classical SIR Model in EBM and ABM Formalism

The first experiment show that we can easily modeling the classical SIR in form of equation-based and also agent-based. As in the Fig. 6, an differential equation can be declare with two expression. The first one on the left of "=" is the keyword diff followed by the name of integrated variable and the time variable t:

```
diff( <integrated variable>, t ) = <calculating expression>;
```

An EBM is then represented as a attributes of agent with a block of equations:

```
equation <name_identifier> {
    diff(...) = ...;
    diff(...) = ...;
    ...
}
```



$$\begin{cases} \frac{dS}{dt} = -\beta \frac{SI}{N} \\ \frac{dI}{dt} = \beta \frac{SI}{N} - \gamma I \\ \frac{dR}{dt} = \gamma I \end{cases}$$

```
equation SIR{
diff(S,t) = (- beta * S * I / N);
diff(I,t) = (beta * S * I / N) - (gamma * I);
diff(R,t) = (gamma * I);
}
```

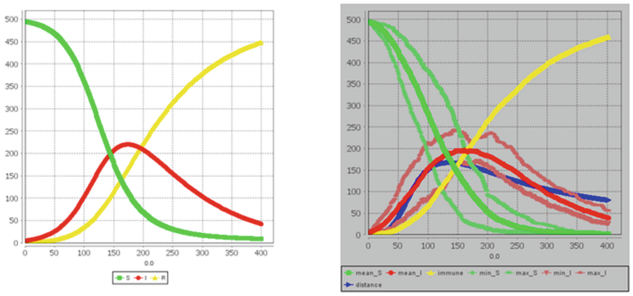
Fig. 6. Representation of an equation-based model in an simulation platform.

5.3 Adjust the Parameters to Calibrate EBM and ABM

The ABM simulation result is a stochastic result, instead of EBM'results are deterministic. Our proposition allow modeler to calibrate the SIR model in ABM fit with EBM. We launch the simulation with following parameter: N = 500; I = 1.0; S = N - I; R = 0.0; beta = 1/2.0; gamma = 1/3.0. After 100 simulations, the SIR model and agent model present significant differences from (Fig. 7): population initial (N), effect of size grid (grid size), effect of topologies (neighborhood size).

The transition beta from EBM to ABM is then adjust an amount alpha. We relaunch the simulation 100 times to explore the value of alpha. We found the best fixed alpha = 0,45 (Fig. 8). We have also found several criteria that would be effect the fitness between SIR EBM and ABM are: difference of synchronous/asynchronous (infect others vs is infected); random walk; effect of beta; dispersion; effect of movement speed.

$$\beta_m = \beta \frac{\textbf{neighborhood size}}{\textbf{grid size}} \mathbf{N} \times a \quad , a \text{ adjustment parameter}$$



Adjusted math model

a = 0.45

ABM models

Fig. 7. Calibrate the beta parameter of SIR model of Switch model by adjusting an alpha parameter.

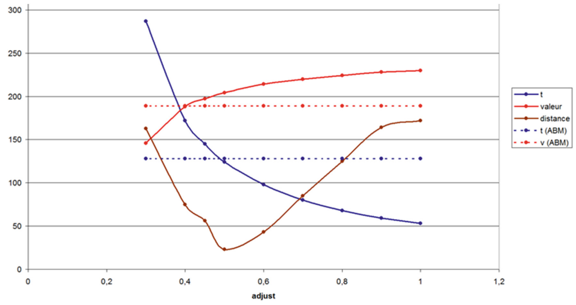


Fig. 8. Adjust the alpha parameter of SIR model to calibrate EBM with ABM result.

5.4 Regenerate Spatial Information from EBM to ABM

In this experiment (Fig. 9), we save the attributes, especially the location and the contamination status of all agents when we do a switch from ABM to EBM model. Then when re-assign to agents. The image represent the regeneration algorithm in order: (a) (e) step 0, (b) (f) before the switch, (c) (g) after the generation, (d) (h) step 100. The (a) (b) (c) (d) take the seed of random 0.123. The (e) (f) (g) (h) have the seed 3.14.

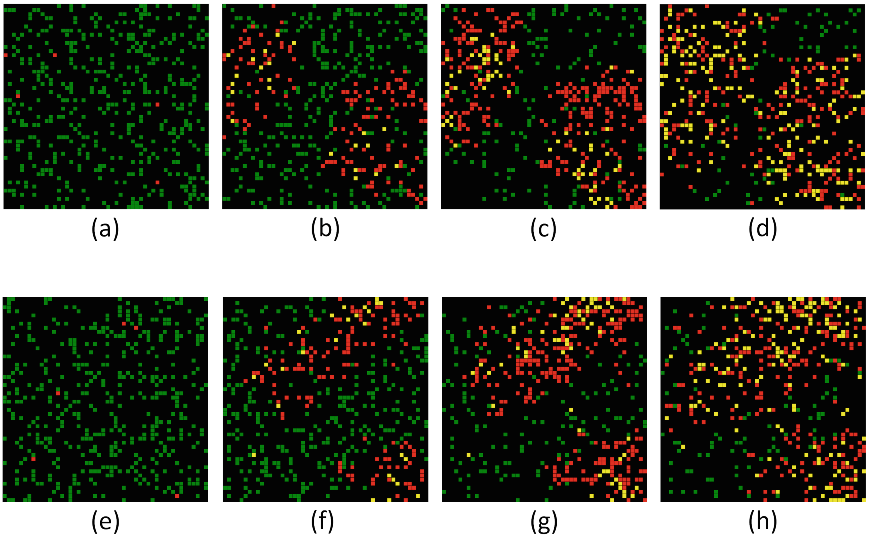


Fig. 9. Regeneration of spatial information algorithm.

6 Conclusion

This paper has proposed a hybrid approach combining modeling equations and agents, as well as its implementation on the modeling platform Gama. We are interested in the representation of this approach theoretical epidemiological models. We illustrate the construction of a class of models based on a SIR model in which people are represented by agents when their density is low, and equations with higher density, a tilt mechanism for moving from an approach to the other. We compare this model with existing models and present a method to determine the parameters during transitions between models. In particular, we seek to establish a link between the parameters of the mathematical model and representation of contacts and travel agents in a spatial environment. We are also interested in how to compensate the loss of information on spatial structures when moving an agent model to a mathematical model.

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