An Ontological Model for the Annotation of Infectious Disease Simulation Models

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Abstract. In this paper, we propose a conceptualization of knowledge of infectious disease simulation models. This model is intended to annotate a set of qualitative and quantitative simulation models to automate their composition in a process of simulation of the spread of infectious diseases. We propose a use case illustrating the use of the ontological model for the annotation of two schistosomiasis simulation models.

Keywords: Ontology · Annotation · Composition · Simulation model · Infectious disease · Schistosomiasis

1 Introduction

In the study of complex social and natural phenomena, it is sometimes necessary to combine several dynamics or several points of view of a system to correctly understand its functioning and its evolution [1, 2]. Thus, the modelers of these systems are more and more confronted with the difficulties of representing them with a single model. In addition, they generally rely on multidisciplinary theories and use different modeling approaches to represent these subsystems. This often results on the one hand, in having several heterogeneous models for the same system; and on the other hand, the necessity to compose these different models in order to better understand this system [3].

In addition, the process of simulating a behavior of these multi-model systems is in itself a delicate exercise that requires the ability to identify, compare, and select models that can answer the question behind a simulation; then, if several models are selected, to assemble them and to integrate data and applications needed to perform the simulations.

In this work, we are interested in the field of infectious diseases and in simulation models of their underlying dynamics. It's a work that aims to set up an ontology-based platform to automate the simulation process of infectious disease models. The purpose of this article is therefore to propose a conceptualization of the knowledge of these models. The resulting ontology will serve as a basis for annotating a set of qualitative and quantitative simulation models for infectious diseases.

G. Bassioni et al. (Eds.): InterSol 2019, LNICST 296, pp. 82–91, 2019.
https://doi.org/10.1007/978-3-030-34863-2_8

After presenting the context of our work in Sect. 2 of this paper, we present in Sect. 3 some related works. Section 4 proposes a taxonomy of knowledge of infectious disease simulation models on which the ontology we propose in Sect. 5 is based. Section 6 presents a use case of two simulation models of schistosomiasis annotated with this ontology.

2 Context

The field of an infectious disease spread can be divided into two subdomains: the subdomain of the disease (its transmission mechanism within a population, the various entities included in it and their relationships) and the sub-domain of risk factors (the set of socio-economic, environmental, biological and behavioral elements, that may influence the spread of the disease) [3, 4]. In each of these subdomains, we can identify a set of underlying dynamics. For example, concerning schistosomiasis, its transmission mechanism is often described according to two dynamics: intra-host dynamics (which gives the evolution of the pathogen inside the host organism) and extra-host dynamics or infection dynamics (which ensures the passage of the pathogen from one host to another). The dynamics of access to infectious water, based on a set of socio-economic factors, is also crucial [5]. Each of these dynamics is in itself a complex phenomenon involving several heterogeneous entities of different natures and sizes, also evolving in different environments.

Conceptually, we can see the propagation of an infectious disease as a system with several levels of interactions, which can be located at different spatial and temporal scales (see Fig. 1).

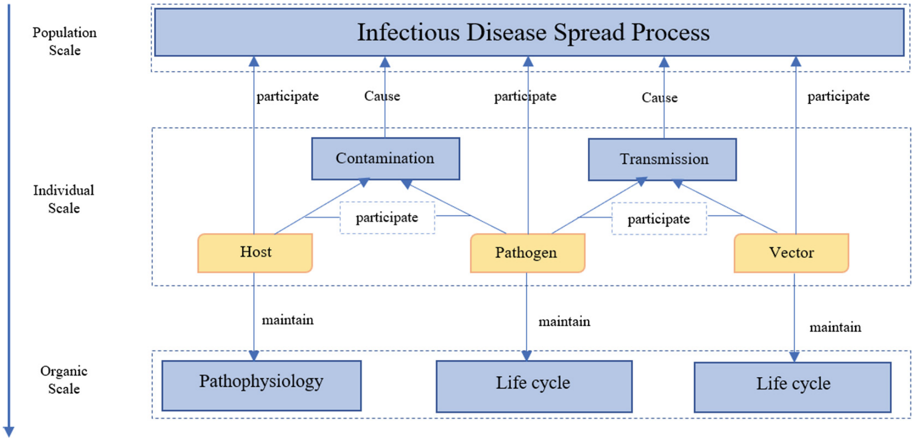


Fig. 1. Scales of infectious disease spread process

This point of view reveals two important things: the difficulty (see the impossibility) of having a single model that represents all these levels of interaction and the possibility to model a level or a set of levels while ignoring the others [3, 5].

The specific problem that interests us in this work is that of the spread of schistosomiasis in Senegal. In recent years, it has been studied by several teams of researchers working in different fields of research: biology, epidemiology, biomathematics, bioinformatics… For this, there is currently a variety of models on schistosomiasis. These models are established on the basis of different modeling approaches and multiple objectives, targeting particular levels of interaction, manipulating heterogeneous data and simulated in dedicated platforms. The ontology we propose allows annotating these different models and their associated simulation platforms.

3 Ontology and Simulation Models

Ontologies are interested in representing the knowledge of a domain. They consist more precisely in the identification of concepts and their relations, and in proposing their formal representation for resource annotation and semantic reasoning [6–8]. Based on these representations, an autonomous agent will have the ability to understand and effectively manage a system, reason and make deliberations.

In recent years, the modeling and simulation community has been using ontologies to improve and facilitate the framework of his work.

Ontologies are used in modeling and simulation as a qualitative approach to represent complex systems. This ontology-based modeling approach is often used to overcome the limitations of numerical modeling approaches: difficulties in obtaining numerical data to conduct simulations; difficult to compose or integrate a set of numerical models due to the varieties of formalisms (differential equations, multi-agent system, etc.) used to represent them. Ontology-based models allow representing the possible behaviors of a system from the abstract description of its internal processes and its different states. Thus, on the basis of a qualitative reasoning, they allow making deliberations without the necessity of certain numerical data [4, 9, 10].

Otherwise, ontologies are used in the process of modeling and simulation, in a framework called "Ontology Driven Simulation (ODS)". It is a process that uses the knowledge encoded in ontologies to dynamically and automatically design simulation models. It's about having, on the one hand, the ontologies of the domain or the application and on the other hand, the ontologies of modeling (encoding information on the modeling such as components of the models, the different phases and modeling activities, etc.). Then, domain ontology concepts are mapped to the concepts of modeling ontologies, then instances of modeling ontologies are created to represent a model. Once ontology instances representing the model are created, additional tools are used to translate them into an executable simulation model [11, 12].

Other works go further in the use of ontologies in modeling and simulation. This is the case of works that use ontologies to drive the integration of models and interoperable simulation applications. In the process of application integration, there are two main difficulties that have been until now technical limitations for the modeling community: semantic accessibility, caused by the inability to explicitly specify the semantics of information contained in different applications; and logical disconnection, caused by the inability to explicitly represent constraints related to the information contained in different applications [12, 13]. In these latest articles, the authors show how to use ontologies to overcome these technical limitations and facilitate the integration of interoperable applications.

In [14], authors use ontologies to assemble semi-automatically, simulation models of an industrial installation composed of a set of hardware devices. Indeed, in this industrial system, each device (composed of a set of devices) is simulated by selecting one or more models. To automate this task, the authors propose an ontology of the industrial plant and its various hardware devices, an ontology of the library of simulation models used to simulate the devices of the industry, a mapping ontology between devices and simulation models and a semantic engine that, from a given hardware device, selects and assembles (if necessary) the models necessary for its simulation.

4 Taxonomy of Simulation Models of Infectious Diseases

In the study of infectious disease simulation models, we identified different types of model categories. This typing is due to the fact that one can consider different points of view, considering them as “keys of determination”, to categorize the simulation models of diseases. A useful way of constructing taxonomy of models is to establish subsumption relations between the elements of these different viewpoints.

First point of view – the models are categorized according to the three dimensions (scales) considered in the spread of infectious diseases (organic scale-lower scale, individual scale and population scale-higher scale). It is the **dimensional categorization** of simulation models of infectious diseases.

Second point of view – the models are categorized according to their objective functions (modeling objectives). It is the **functional categorization** of simulation models of infectious diseases.

Third point of view – the models are categorized according to the modeling techniques and formalisms used. It is the **technical categorization** of simulation models of infectious diseases.

Thus, any simulation model of an infectious disease must be identified according to these different types of categories. We give below the details of each categorization.

4.1 Dimensional Categorization

A description of infectious disease models is given by considering three dimensions (scales):

- Population scale: in this dimension, models focus on the spread of diseases, on the populations of actors included (populations of final hosts, intermediate hosts, populations of pathogens, vector populations, etc.) and on the factors involved. We found here models of transmission dynamics or epidemiological models. They are two categories: epidemiological models of transmission and geographical models.

Epidemiological Models of Transmission (**EMT**) relate to variations in infection rates in human hosts and vectors. There are several types of epidemiological models of transmission: **SI**, **SIR**, **SIER**, etc. Geographic Models (**GEM**) are epidemiological models that incorporate environmental factors and describe the spatial distribution of diseases or vectors [15].

- Scale of individuals: in this dimension, models focus on individuals in a particular population and consider their actions and interactions with, sometimes, components of other populations or other influential factors. We found here models of population dynamics (population of pathogens - **MPP**, vector population - **MVP**) which mainly deal with genetic aspects of pathogen dynamics with sometime, human and vector host components and/or an epidemiological component (i.e. the level of transmission) [16]. One found here also models of host-to-host contamination or pathogen transmission (**MC**) [3, 4].
- Organic scale: in this dimension, models look at pathophysiological processes. One found here Intra-host models (**MIH**) that generally describe the dynamics of parasite larval stages and its interactions with body organs and the immune system [17]. They also study their interactions with drugs and the effects of medicinal treatments in pest biology [18].

4.2 Functional Categorization

A categorization of models is given considering the problems posed or the modeling objectives (their objective functions). Generally, simulation models of infectious disease can be classified into two broad categories: predictive models, also called behavioral models and understanding models, also called models of knowledge [16].

Predictive models (Prediction function) are models of “black box” types, built on the basis of quantitative and/or qualitative data only, expressed as input and output parameters. There are several types of predictive models depending on the possible objectives: simulation models (**Simulate**: simulate the spread of a disease in a given population, simulate the behavior of a pathogen, etc.), prediction models (**Predict**: predict the spread of an epidemic after the occurrence of an event, etc.), evaluation models (**Assess**: evaluate or estimate the impact of a control strategy, assess the role of the geographic dimension in the distribution of a disease, etc.).

Knowledge models (**Comprehension** function) are constructed on the basis of assumptions that are often sought to confirm or refute, or that are used to understand certain aspects of diseases.

4.3 Technical Categorization

A categorization of models is given here by considering the techniques and formalisms used to model the dynamics of infectious diseases. Mainly, we can consider two broad categories of simulation models: numerical models (or quantitative models) and analytical models (or qualitative models).

Numerical models (**Quantitative**) are built on the basis of quantified numerical data. Among these types of models, there are mathematical models based on equations (**EBM**) and agent-based models (**ABM**).

Qualitative models (**Qualitative**) attempt to explain in a qualitative way, without certain numerical data, the phenomena. Among this type of models, there are ontology-based models (**OBM**), cellular automaton-based models (**CABM**), and so on.

5 An Ontology of Infectious Diseases Simulation Models

The ontology that we propose here will allow annotating simulation models of infectious diseases. It is based on the taxonomy proposed in the previous section (illustrated in Fig. 2) and includes other elements related to parameters (**Parameter**), hypothesis (**Hypothesis**), actors (**Actor**), objects (**Object**) and activities (**Activity**) taken into account in the model, as well as the implementation language (**Language**) and simulation platform (**Platform**) used. Other elements related to the identification of models are also added: model ID (**ID**), authors of the model (**Author**), its publication journal (**Journal**), the publication title of the article (**Title**) and a short description of the model (**Description**).

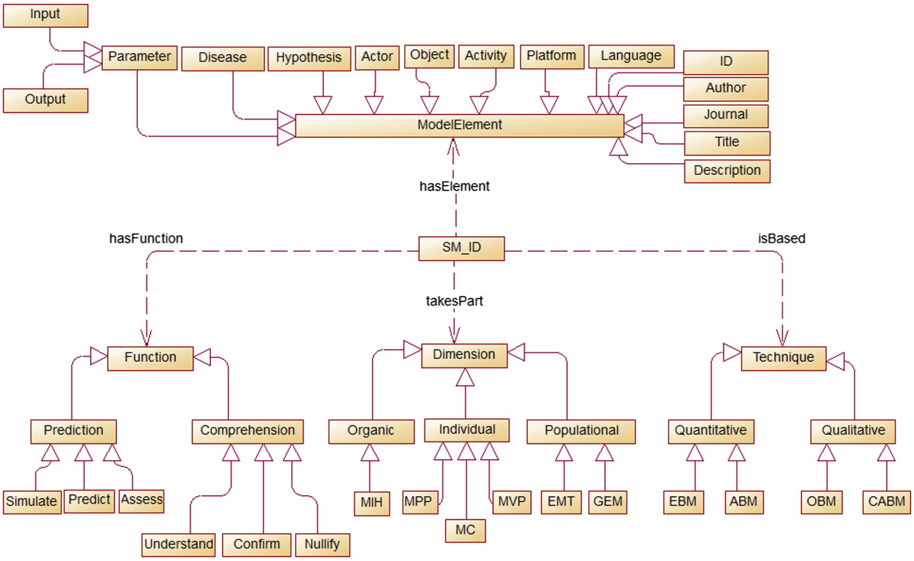
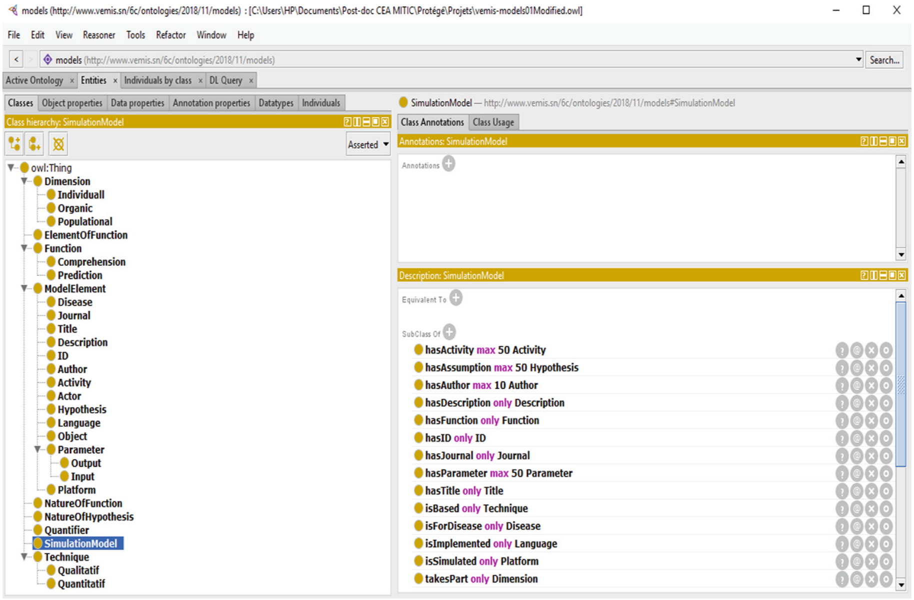


Fig. 2. Ontology of infectious diseases simulation models

This ontology allows describing, in a generic way, any simulation model of an infectious disease by specifying its scale (intra-host, epidemiological, etc.), its objective function (prediction, comprehension, etc.), formalism used (Equations, Agents, Ontology, etc.), elements included (parameters, assumptions, actors, objects of the environment, activities or dynamics implemented, etc.), implementation language and execution platform.

The Fig. 3 is a preliminary OWL formalization of the ontology through Protégé.

To use this ontology for a particular infectious disease (Schistosomiasis, for example), it is necessary to make the mapping between it (**SM-ID**) and the domain ontology of schistosomiasis (***IDOSCHISTO***) [10]. This mapping is ensured by a coupling between these two ontologies which results in the establishment of links between, for example, concepts as **Disease**, **Actor**, **Activity**, **Object**, **Dimension**, etc. in **SM-ID** and the corresponding elements in **IDOSCHISTO**. The resulting ontology (Ontology of Schistosomiasis Simulation Models - **OSM-Schisto**) will thus be able to annotate all Simulation Models of Schistosomiasis.



- owl:Thing
  - Dimension
    - Individuall
    - Organic
    - Populational
  - ElementOfFunction
  - Function
    - Comprehension
    - Prediction
  - ModelElement
    - Disease
    - Journal
    - Title
    - Description
    - ID
    - Author
    - Activity
    - Actor
    - Hypothesis
    - Language
    - Object
    - Parameter
      - Output
      - Input
    - Platform
  - NatureOfFunction
  - NatureOfHypothesis
  - Quantifier
  - SimulationModel
  - Technique
    - Qualitatif
    - Quantitatif

hasActivity max 50 Activity
hasAssumption max 50 Hypothesis
hasAuthor max 10 Author
hasDescription only Description
hasFunction only Function
hasID only ID
hasJournal only Journal
hasParameter max 50 Parameter
hasTitle only Title
isBased only Technique
isForDisease only Disease
isImplemented only Language
isSimulated only Platform
takesPart only Dimension

Fig. 3. The ontology formalization with Protégé editor

6 Use Cases

6.1 Use Case 1 (See Table 1)

This simulation model [19] is a transmission model of schistosomiasis taking into account heterogeneities. The authors calculate the basic reproductive rate R_0 in order to pronounce on the disease-free equilibrium which is globally asymptotically stable if $R_0 < 1$; and on the disease-endemic equilibrium which is globally asymptotically stable if $R_0 > 1$.

Table 1. First simulation model annotated.

Concept	Instance
Function	Simulate
Dimension	Epidemiological model of transmission
Technique	Numerical: based-Equation
Language	ODE
Platform	Scilab
Actor	Human Population; population of mollusk
Object	Geographical sites: residential (village), water points (pond, river, pond)
Activity	Agriculture, travel
Input parameter	Human population, number of pools, number of dwellings (villages)
Output parameter	Basic reproduction rate

6.2 Use Case 2 (See Table 2)

This simulation model [20] is a transmission model that aims to assess the spatial impact on schistosomiasis control policies. Three control policies are considered: treatment of infected individuals, elimination of cercariae and elimination of mollusks. The authors calculate the evolution of infections by applying different spatial configurations with each of these three control policies with.

Table 2. Second simulation model annotated.

Concept	Instance
Function	Assess
Dimension	Epidemiological model of transmission
Technique	Numerical: Agent-based
Language	GAML
Platform	GAMA
Actor	Human population (man, woman, child); mollusc population; pathogen
Object	Geographical sites: residential (village), water points (pond, river, pond), roads, schools
Activity	Fun, housewives, and professionals activities; treatment of individuals, elimination of mollusks, elimination of cercariae
Input parameter	GIS of the studied area (dwellings, water points, roads, schools), human populations, mollusks and pathogens
Output parameter	Evolutions of the spread of the disease

7 Conclusion and Perspectives

In this paper, we have proposed a core ontological model for annotating quantitative and qualitative simulation models for infectious diseases. We highlighted the main concepts and there relations. Use cases are presented for illustrating how the ontological model could be used for annotating existing simulation model for schistosomiasis disease.

Our future work will first focus on finalizing the formalization and the validation of the ontology. Second, we will implement the ontology-based library, a web platform, for hosting infectious diseases simulation models and their metadata. Then, we will set up a semantic engine that, based a user request, will autonomously orchestrate the simulation process. The orchestration of the simulations consists first of choosing the type of model (numerical or qualitative), then selecting the simulation models to compose and finally integrating the data and the applications necessary for the realization of a simulation.

Acknowledgements. This work is supported by the African Center of Excellence in Mathematics Computer Science and ICT (CEA-MITIC) through a postdoctoral contract within the VEMIS project (Infectious Disease Epidemiological Monitoring in Senegal).

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