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A FRAMEWORK FOR MODELING AND SIMULATING *Aedes aegypti* AND DENGUE FEVER DYNAMICS

Tiago Lima
Tiago Carneiro
Leandro Silva

Federal University of Ouro Preto (UFOP)
Ouro Preto, MG, BRAZIL

Raquel Lana
Cláudia Codeço
Izabel Reis

Oswaldo Cruz Foundation (Fiocruz)
Rio de Janeiro, RJ, BRAZIL

Raian Maretto
Leonardo Santos
Antônio M. V. Monteiro

National Institute for Space Research (INPE)
São José dos Campos, SP, BRAZIL

Liliam Medeiros

São Paulo State University (UNESP)
São José dos Campos, SP, BRAZIL

Flávio Coelho
Getúlio Vargas Foundation (FGV)
Rio de Janeiro, RJ, BRAZIL

ABSTRACT

Dengue fever represents a great challenge for many countries, and methodologies to prevent and/or control its transmission have been largely discussed by the research community. Modeling is a powerful tool to understand epidemic dynamics and to evaluate costs, benefits and effectiveness of control strategies. In order to assist decision-makers and researchers in the evaluation of different methodologies, we developed DengueME, a collaborative open source platform to simulate dengue disease and its vector's dynamics. DengueME provides a series of compartmental and individual-based models, implemented over a GIS database, that represents the *Aedes aegypti*'s life cycle, human demography, human mobility, urban landscape and dengue transmission. The platform is designed to allow easy simulation of intervention scenarios. A GUI was developed to facilitate model configuration and data input.

1 INTRODUCTION

Controlling dengue fever is a public health challenge. This disease presents a complex dynamic, governed by the interaction of multiple agents as humans, mosquito vector (*Aedes aegypti*) and dengue virus, in a complex space. The assessment of the alternative control strategies such as spatially localized chemical treatments to reduce mosquito density requires computer-simulated scenarios to optimize the allocation of resources. Modeling the transmission dynamics of dengue fever is also a powerful tool for evaluating vaccine programs (Rico-Hesse 2010, Luz et al. 2003).

Meteorological variables, such as temperature, rainfall and humidity, interfere in all developmental stages of the dengue vector, from egg viability to the longevity and dispersal of adults (Luz et al. 2008, Maciel-De-Freitas, Codeço, and Lourenco-de Oliveira 2007, Honório et al. 2003, Focks et al. 1993, Rueda et al. 1990, Parker 1986). A proper tool for dengue modeling should allow easy incorporation of meteorological data.

Social and demographic changes have also contributed for increasing dengue fever incidence (Gubler 2002, Tauil 2001). The unplanned urbanization together with high human population density lead to the accelerated spread of the disease (McMichael 2004); the precariousness of garbage collection systems and water supply favor the proliferation of mosquitoes breeding sites (Carbajo, Curto, and Schweigmann 2006, Lazcano et al. 2006, Luz et al. 2003), air and land transportation also facilitate the spread of viruses and vectors, as they allow fast displacement of infected people and *Aedes aegypti* eggs between different regions. Incorporate such variables in models requires sub-models to describe the urban landscape and the mobility of individuals through it.

Several models have been developed aiming at understanding the dengue vector population dynamic and spread (Yang and Ferreira 2008, Otero, Solari, and Schweigmann 2006, Otero, Schweigmann, and Solari 2008, Lana et al. 2011), as well as the disease transmission dynamic (Santos et al. 2009, Pinho et al. 2010, Medeiros et al. 2011). However, in general they represent homogeneous populations and scaling them up to several populations (metapopulation models) or introducing spatial heterogeneity demands a high dosage of efficient programming. In this context, this work presents the conception and current development stage of the DengueME (Dengue Modeling Environment) framework, an open source tool aiming at supporting the development and simulation of spatio-temporal models of dengue and its vector, integrated with a GIS.

The DengueME was developed as a tool for helping the designing of site-specific and population-specific control strategies for dengue. To reach this goal, DengueME provides (i) a collection of built in models that can be combined to represent different scenarios; (ii) a modeling language that accommodates both population models and individual-based models, (iii) a friendly graphical interface for easy model choice and configuration; (iv) a flexible and extensible architecture to allow contribution from users, and (v) a standard format for data exchange to allow the communication between DengueME models.

2 MOTIVATION

Computational models have been developed not only for epidemic outbreaks prediction, but also to enable a better understanding of the dynamics of dengue infection transmission, and to analyze the impact of control strategies (Rico-Hesse 2010, Luz et al. 2003). Figure 1 shows the exponential growth of scientific articles on dengue fever in general (blue circles) and articles on dengue models (red squares), in the last two decades (searching the ISI - Web of Knowledge). The growth rate of articles on dengue models is higher than the articles on dengue in general. This scenario illustrates the demand (opportunity) for frameworks that enable fast implementation, selection and testing of alternative dengue models in a single environment.

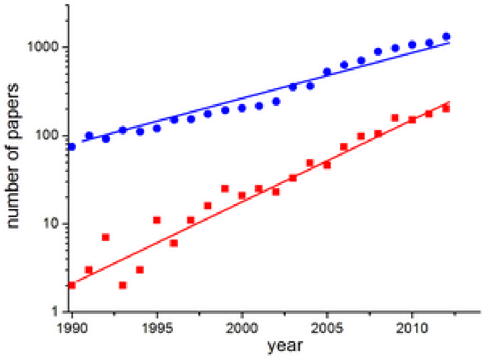


Figure 1: Exponential evolution of publications on dengue (blue circles) and specifically on dengue models (red squares) in the last two decades (search done in ISI - Web of knowledge database).

There are other initiatives to support users on studying environmental phenomena through computer modeling and simulation. Examples include platforms that allow model building by visual metaphors (eg. diagrams) and interacting with graphical interfaces (North et al. 2005, Lima et al. 2013, Tisue and Wilensky

2004, Muetzelfeldt and Massheder 2003). Despite the existence of generic frameworks for modeling disease spread on the global scale such as STEM (Ford, Kaufman, and Eiron 2006) and GLEAM (Balcan et al. 2010), or spread on a connected networks like EpiFire (Hladish et al. 2012), we did not found solutions freely available dedicated to dengue modeling and targeting local dynamics at intra-urban scales.

3 DengueME FRAMEWORK OVERVIEW

DengueME is a software framework for modeling and simulating spatio-temporal dynamics of dengue fever and its vector, *Aedes aegypti*. It provides services to support the development of integrated models and evaluation of intervention scenarios. In the following, the DengueME requirements, design, and current development status are presented.

3.1 Framework Requirements and Design

To meet the proposed objectives, a framework for dengue modeling should offer a basic library of epidemiological (disease transmission) and entomological (mosquito population dynamics) spatiotemporal models. These models should be configured and parameterized to meet the needs of the user and applied to real case studies. In the current version, models developed by Medeiros et al. (2011) and Lana et al. (2011) were adapted to allow easy integration with a geographical database. DengueME models can be implemented in multiple spatial scales and multiple modeling paradigms, including differential equations, agents, cellular automata and hybrids, illustrating the versatility of the framework. Models are implemented using the high level programming language TerraML (Terra Modeling Language) from TerraME (Carneiro et al. 2013). DengueME is an extension of TerraME, a platform for modeling and simulating of environmental systems.

The parameterization and configuration of DengueME models can be directly done using the TerraML programming language. However, to facilitate and improve its usage by people with little programming experience DengueME provides a friendly graphical user interface for customization of different models and intervention scenarios. For this, a Visual Development Environment was built, allowing users to configure models and create scenarios through selection and integration of sub-models (modules) from the framework's library, and parameterize them using data from geographic databases or files containing time series and tabular data.

Furthermore, a dengue modeling framework should enable adding of new models to its library of models in order not to limit its application, allowing for continuous updates and collaborative development. New models can be added as a module (or a black-box) to the DengueME Framework, consisting of: (i) the model, implemented in TerraML and (ii) a XML file which describing its parameters (eg. type and format), inputs and outputs.

The DengueME framework defines a process that uses and produces custom models defined by users. This process is a sequence of steps that are divided into activities which can be performed with the help of specialized tools. The following steps are part of this modeling process: (1) model building phase, (2) sensitivity analysis phase, (3) calibration phase, (4) validation phase, (5) projection scenarios phase. The Model Building phase involves model design, model selection, and data input. The scenario projection phase includes model parameterization, scenario definition, customizing the simulation output, and running the model. Some resources to assist doing phases 2, 3 and 4 are still being developed. Partial results can be found in (Fraga et al. 2010, Silva, Lima, and Carneiro 2011). The detailed presentation of the modeling process is out of scope of this article.

Figure 2 presents an overview of the DengueME framework architecture. In the lower layer, is the TerraME platform for environmental modeling, used to build the models. The second layer is the DengueME framework, composed by a set of models and a middleware to integrate them. Then, we have the layer formed by the models and scenarios customized by the user. They can be developed using the DengueME Visual Development Environment available on the top layer of the architecture. This development environment has a graphical user interface.

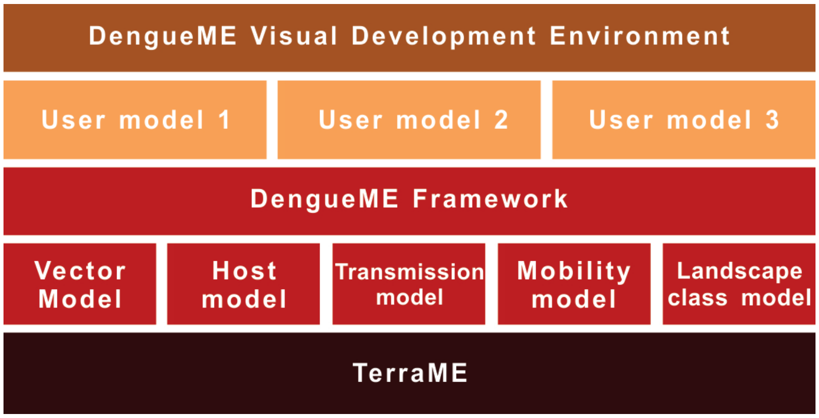


Figure 2: DengueME architecture.

3.2 Models

The transmission dynamics of dengue is governed by the complex interaction between humans, mosquitoes, viruses, on a heterogeneous landscape. The modularization of this dynamics into independent components allows the user to work on different levels of detail and complexity, according to his goals. In the following section, the model components of DengueME are presented (Figure 2).

3.2.1 Vector Models

The vector (entomological) model is a system of differential equations that describes the population dynamics of *Aedes aegypti*. The temporal variation of the stock of individuals in each life stage (eggs, larvae, pupae and adults) is modeled as a function environmental carrying capacity and the climate (Lana et al. 2014). The DengueME framework facilitates building metapopulational models from this basic component, with easy parameterization from a georeferenced database. The vector model can be used stand alone, or integrated with the other models. An example is presented in Section 4.1.

3.2.2 Host Models

The host (human) model is another basic component that can be used stand alone or as part of an integrated model of dengue. It describes the demographic dynamic of the human population in the study area. Census data can be used for spatial allocation of individuals by age, sex or other attributes, into a regular grid, also defined by user. This allocation is done by distributing the population per unit area (neighborhoods or census sectors). Host models can be implemented as differential equations describing the stock of individuals in each cell of the grid; or as an individual-based model in which each person is an agent with attributes (eg. age, sex) and behaviors or rules (eg. movement, susceptibility to infection). The latter is currently implemented on DengueME (see in Section 4.2).

3.2.3 Transmission Models

The virus transmission process between humans and mosquitoes depends on the local amount of susceptible people (or mosquitoes) and infected people (or mosquitoes). Immune people act as barriers to transmission, since they absorb some of the bites from infected mosquitoes, without subsequent spread of the virus. Dengue models describe this dynamic through the classification of the stock of people in four states: susceptible, exposed, infected and recovered. The mosquitoes (adult females) are classified in susceptible, exposed and infected states (they do not recover). In the case of circulation of multiple viral types, these compartments are multiplied (dengue is caused by four distinct virus serotypes). Currently the DengueME framework supports the transmission model considering only one virus type (see example in Section 4.2).

3.2.4 Mobility Models

Another component of DengueME is the mobility model, which describe the mobility and commutation of humans and vectors. The spread of viruses and vectors is facilitated by the flow of individuals through the network of air and land transportation. The human mobility component can be implemented as a unstructured model (no mobility or random mobility at pre-defined intensity) or a structured model based on more complex structures inspired by the actual data (Santos et al. 2009, Santos et al. 2011). Currently, mobility models for humans and mosquitoes available in DengueME are based on those describe by Medeiros et al. (2011) which introduces distinct commutation of individuals between public and private areas.

3.2.5 Landscape Class Models

The urban landscape interferes in the dynamics of dengue transmission as it introduces heterogeneity in the availability of breeding sites for *Aedes aegypti*. The landscape component provides a landscape classification model to describes the space and can be used to obtain input parameters to be used in the models. Landscape classification can be implemented in a very sophisticated way involving techniques for segmentation and classification of satellite images of high spatial resolution, and data mining. DengueME implemented the landscape classification model suited to dengue issues developed by Reis (2010).

3.2.6 Model and Scenario Development Process

DengueME was designed to facilitate usage by those with no programming knowledge. The DengueME Visual Development Environment implements services to help users to perform the required steps for developing models and defining scenarios. Its GUI provides wizards that guide users in performing the steps along the process, as shown in Figure 3. It allows users to select the set of models to be used and the way they will be integrated; to provide the parameters for each model; to set the options for output visualization and storage. The user defined settings and parameters (designed scenarios) can be stored and retrieved for later use. After finishing all customization and parametrization, the GUI allows the generation of the corresponding TerraML source code.

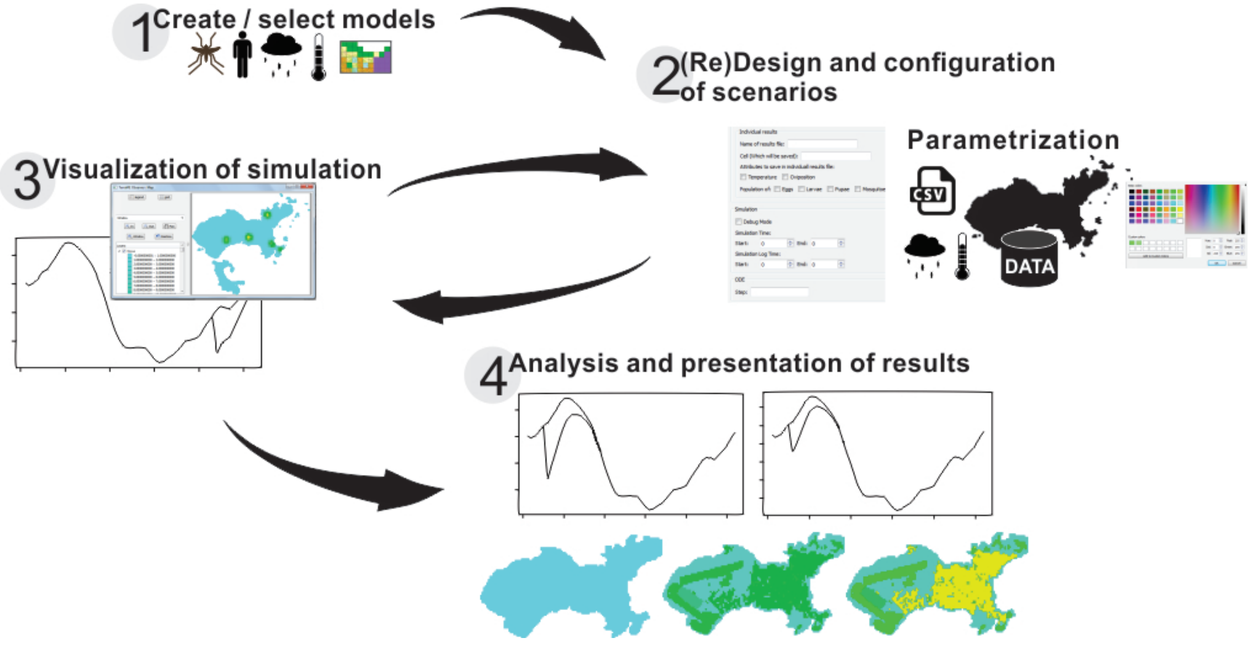
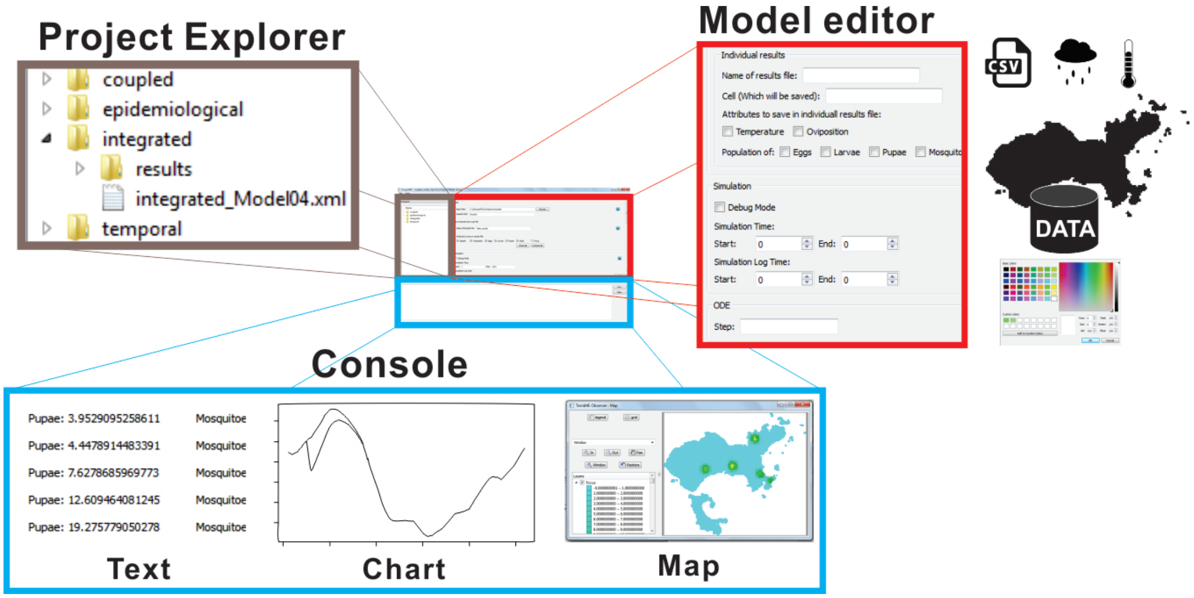


Figure 3: Diagram showing the modeling process using the DengueME Visual Development Environment.

3.3 DengueME Visual Development Environment

The GUI components of DengueME Visual Development Environment are presented in Figure 4. The goal is to eliminate barriers related to using programming languages and facilitate the framework utilization. Its design works with the concepts of Workspace (working directory that contains the user's projects), View (interface components for browsing and / or presenting information on projects and models), and Editor (interface components for editing models). Figure 4 illustrates some of these features: (a) the Project Explorer displays and allows navigation through projects and existing models within the workspace, (b) the Model Editor allows setting of model's parameters and scenarios (eg. using GUI to import meteorological data and also of other types, from .csv text files or databases), as well as the output options, (c) the Console view presents information and views derived from the simulations.



Individual results
Name of results file:
Cell (Which will be saved):
Attributes to save in individuall results file:
☐ Temperature ☐ Oviposition
Population of: ☐ Eggs ☐ Larvae ☐ Pupae ☐ Mosquito

Simulation
☐ Debug Mode
Simulation Time:
Start: 0 End: 0
Simulation Log Time:
Start: 0 End: 0

ODE
Step:

```
Pupae: 3.9529095258611      Mosquitoe
Pupae: 4.4478914483391      Mosquitoe
Pupae: 7.6278685969773      Mosquitoe
Pupae: 12.609464081245      Mosquitoe
Pupae: 19.275779050278      Mosquitoe
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Figure 4: Graphical interface of the DengueME Visual Development Environment.

4 DengueME APPLICATION

The following sections describe the application of DengueME in real world case studies.

4.1 Using DengueME to Evaluate the Impact of Local Interventions on Dengue Vector Density

DengueME can be used to explore the impact of locally applied intervention strategies on the local and global density of *Aedes aegypti* allowing comparison between different scenarios. Ilha do Governador, an island in Rio de Janeiro city, Brazil, was used as study area (Figure 5). The map of census tracts, obtained from IBGE (Brazilian Institute of Geography and Statistics, 2010) was used to define the regions for adulticide application. The pink area in Figure 5(b) was chosen to simulate the intervention, due to its denser human population. Figure 5(c) shows the three quadrants where the ultra-low volume adulticide, with maximum efficacy of 0.9 and an average persistence of one day, was applied.

Figure 6(a) shows the output of DengueME, showing the impact of the intervention at the scale of the whole island. Figure 6(b) shows the impact of this application in the local population. At the global scale, the intervention did not present a significant impact. However, at the local scale its impact was significant for a few days. After this period, the population recovered, due to the low persistence of the simulated insecticide and the short period of application.

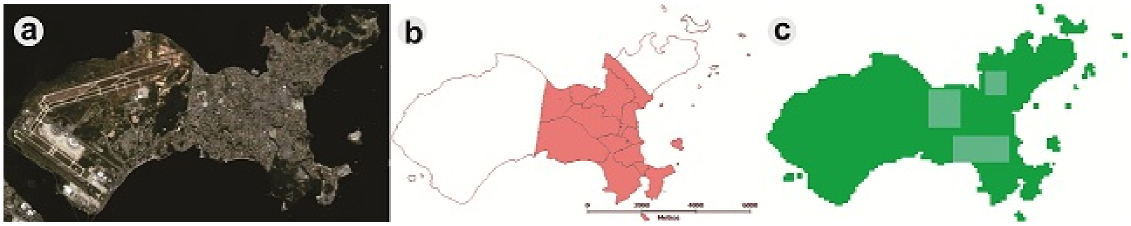

Figure 5: Study area, Ilha do Governador. a) Satellite image (Google Earth). b) Map of census tracts. c) Simulated map generated by DengueME. Highlighted blue areas are sites of application of adulticide.

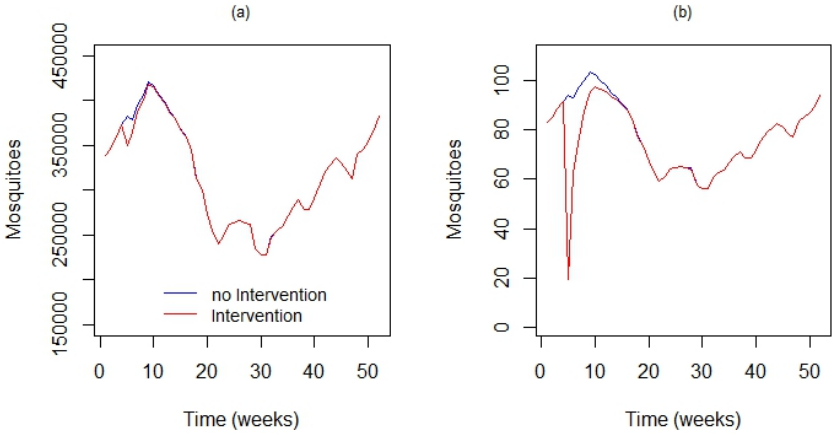

Figure 6: Using DengueME to simulate locally applied chemical interventions. Comparison between the the vector population in the study area with and without application of adulticide. (a) global impact considering the entire study area. (b) local impact in a 100x100m area.

4.2 Using DengueME to Study Epidemic Scenarios

The spatial spread of dengue fever is the result of complex dynamic interactions between humans, mosquitoes and different virus serotypes. To illustrate this dynamic, Figure 7 shows the result of a spatial dengue spread simulation in Ilha do Governador. Epidemic waves travel from the commercial areas to the residential areas of the island. This is an example of the dengue agent based model, adapted from Medeiros et al. (2011), implemented in DengueME. The model was configured to run over a grid of cells with size 100 X 100 meters.

Figures 8(a) shows the time series of susceptible, infected and recovered humans and Figure 8(b) shows the time series of susceptible and infected mosquitoes, respectively, generated by DengueME. Control strategies were not implemented in this experiment, only human and mosquitoes mobility and the virus transmission.

5 DengueME EVALUATION

A first evaluation of the DengueME environment was carried out aiming at identifying the perception of potential users of its applicability and potential use for teaching, researching and decision making supporting activities, as well as help prioritizing future development efforts. To this end, a group dynamic section was implemented during the III Symposium on Modeling Dengue, occurred between 8 and 10 May 2013. The group dynamic section followed three steps: (i) a brief presentation about the framework and its objectives; (ii) participants were invited to install the framework following a guide; (iii) participants did an exercise parameterizing and running built in DengueME models. At the end, they were invited to fill in a questionnaire

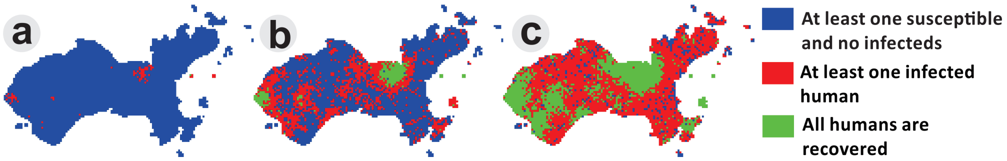

Figure 7: Using DengueME to simulate dengue spread from commercial to residential areas of a city. Panels show three moments of a simulated epidemic in the study area. (a) Beginning of the simulation with a few hotspots; (b) propagation waves from the hotspots; (c) overall dissemination and pockets of immunity.

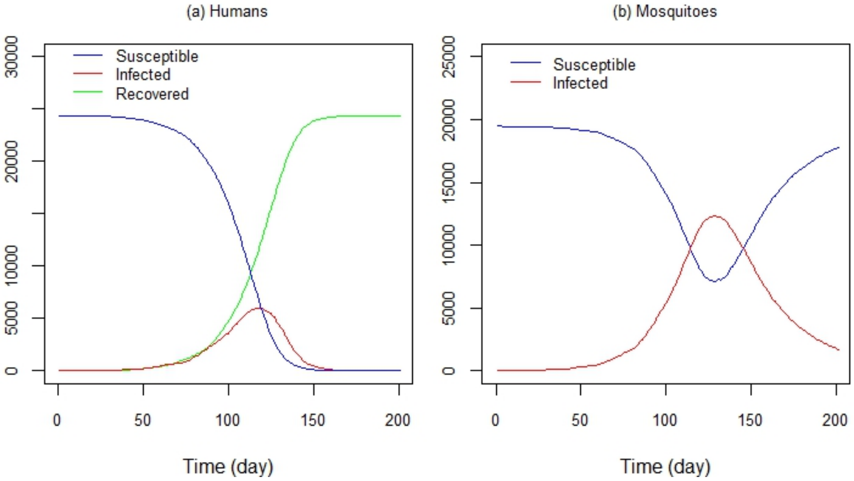

Figure 8: DengueME output. Time series of (a) susceptible, infected and recovered humans and (b) susceptible and infected mosquitoes, genetared by DengueME simulations.

reporting their experience and providing feedback. At last, a focal group was created. Focal group is a technique that allows collecting data about participants' perceptions through a moderated discussion. The study had the participation of 16 individuals with different backgrounds, but mostly university professors and students with several expertise areas (Entomology, Medicine, Epidemiology, Biomedical Engineering, Statistics, Biology, Computer Science, Physics), as well as varied degrees of experience in programming and dengue modeling.

Overall, the results of this group section suggest that the DengueME Visual Development Environment is friendly for building and running models and scenarios. All users completed the proposed tasks, and most of them without help. However, some participants reported difficulty understanding the built in models from the information offered by the development environment. This result indicates the necessity of further investments in documentation. Overall, we concluded that a graphical interface helps model building, and it is an important investment for fostering its use as a tool to support the design of interventions.

An important goal of this study was to identify the applicability and potential use of DengueME in different activities. A large fraction of the participants evaluated positively its applicability potential for supporting research and teaching (Figure 9a). Some participants even manifested interest in using it in classroom and to collaborate with new models. The participants were more divergent when asked about its application as a tool to support decision making (Figure 9b). This could be partly explained by the difficulties found on the current version regarding the available help information required for users to understand the models. Further effort is required to make DengueME more accessible for non expert users (eg. health workers).

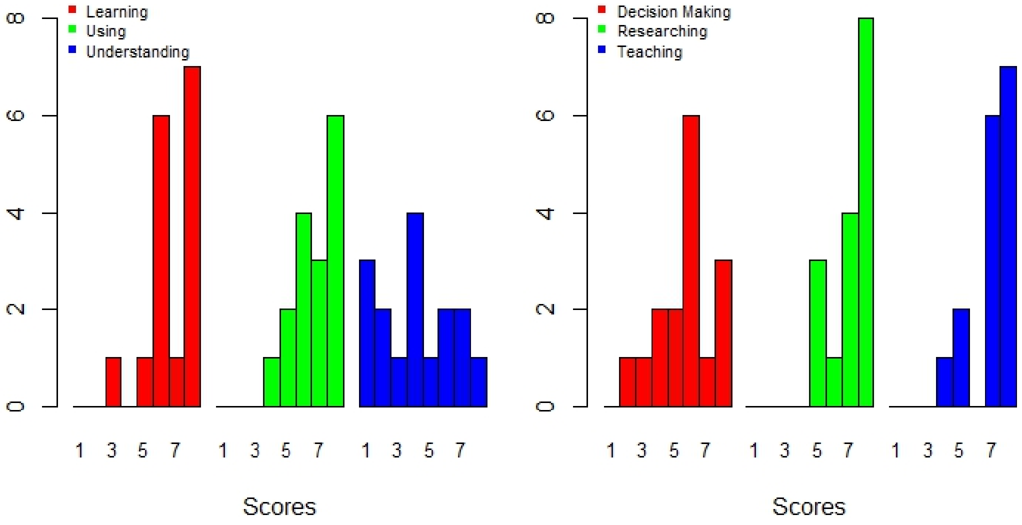

Figure 9: User's evaluation of the current DengueME graphical interface

6 RESULTS

This work describes the implementation and evaluation of a tool for the planning of control strategies for dengue fever - the DengueME framework. Models that have already been calibrated and validated in real case studies were selected from the literature and added to DengueME library. Differences in the modeling paradigms, spatiotemporal scales and set of parameters used in these models stressed the extensibility and flexibility of DengueME software architecture. This experience provides the authors with the necessary feedback to improve the mechanism for model integration through XML files. The visual development environment for models and scenarios was implemented and applied in real case studies. A group of experts on dengue fever control positively evaluated the DengueME framework.

7 FINAL REMARKS

Despite the success of mathematical models in explaining *Aedes aegypti* spatial dynamics and dengue transmission, it is still necessary to encourage their use for the planning of dengue control interventions. The proper use of these models requires the understanding of model assumptions. However, it should not require extensive experience in programming techniques or in model development. Currently, fast model reuse is still a challenge.

In this context, DengueME friendly graphical user interface and wizards allow users to customize models and scenarios from built in modules fitting them to real data. New models can be added to DengueME extensible architecture. By comparing the outcomes of several models users can better understand the ability of each module (and of the modeling paradigm used in it) in reproduce the dynamics and spatial patterns observed in dengue fever datasets.

This work remains under development. Partial results were obtained, analyzed, and positively evaluated, motivating its continuity. Future work includes: (i) develop features for evolution and maintenance of the models library (eg. use of standardized XML schemas for model integration as provided by OpenMI, customized generation of graphical interfaces for new models, web service for software updates). (ii) performing further framework evaluations with potential users, (iii) developing and incorporating new models into the framework, (iv) developing new case studies, (v) providing tutorials and demo applications to support users.

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AUTHOR BIOGRAPHIES

TIAGO F. M. LIMA is Assistant Professor of the Computer and Systems Department at UFOP, where he heads the Laboratory of Engineering and Development of Systems (www.leds.ufop.br). He is graduated in Computer Science (UFOP) and Master in Analysis and Modeling of Environmental Systems (UFMG). His email address is tiagolima@decsi.ufop.br.

TIAGO G. S. CARNEIRO holds a BA, MS and Ph.D. in computer science by Brazilian institutions UFOP, UFMG and INPE. He is associate professor of the Computer Science Department at UFOP, where he heads the Laboratory for Modeling and Simulation of Earth Systems - Terralab. He is the chief developer of TerraME (www.terrame.org), a platform for modeling and simulation of nature society interactions. Currently, he is a visiting researcher associate in the Ecosystems Lab at Oxford, UK. His email address is tiago@iceb.ufop.br.

RAQUEL M. LANA is a PhD student of the Epidemiology in Public Health program in the Oswaldo Cruz Foundation. Her email is raquelmlana@gmail.com.

CLÁUDIA T. CODEÇO is Associate Researcher and Coordinator of the Scientific Computation Program at Oswaldo Cruz Foundation, RJ/Brazil. She holds a Ph.D. in Quantitative Biology from the University of Texas, USA, and develops research on vectorborne disease modeling. Her email address is codeco@fiocruz.br.

RAIAN V. MARETTO is graduated in Computer Science (UFOP) and Master in Remote Sensing (INPE). He is currently a developer at the Center for Earth System Science (CCST/INPE). His email address is rvmaretto@gmail.com.

LILIAM C. C. MEDEIROS is Professor of Mathematics at Environmental Engineering Department at UNESP. She received her M.S. in Mathematics at UFMG and her Ph.D. in Computational Mathematics at UFPE. Her research deals with Modeling in Epidemiology. Her e-mail is liliam.medeiros@ict.unesp.br.

LEANDRO G. SILVA is a undergraduate student in Computer Engineering at UFOP. His email address is leandrogs99@gmail.com.

LEONARDO B. L. SANTOS is graduated in Physics (UFBA), MS and PhD in Applied Computing (INPE). He is currently an analyst on the development division of the Brazilian National Center for Monitoring and Early Warning of Natural Disasters (Cemaden). His email address is santoslbl@gmail.com.

IZABEL C. REIS is a PhD student of the Tropical Medicine program in the Oswaldo Cruz Foundation. She holds biology graduate and M.S in Remote Sense apply to human Health, dengue in the National Institute for Space Research. Her email is izabio2005@gmail.com.

FLÁVIO C. COELHO is an Associate Professor at the Applied Mathematics School of Getulio Vargas Foundation. He received his PhD from The University of Texas at Arlington in 1999. His research interests include the mathematical and computational modeling of infectious diseases. His email address is fccoelho@fgv.br.

ANTÔNIO M. V. MONTEIRO is Researcher of the Division of Image Processing (INPE) and Professor of PhD programs in Applied Computing, Remote Sensing, and Earth System Science. He holds a PhD in Electronic Engineering and Control/Computer Science from the University of Sussex, UK. His email address is miguel@dpi.inpe.br.