[AM-07-084] Simulation Modeling

Abstract

Advances in computational capacity have enabled dynamic simulation modeling to become increasingly widespread in scientific research. As opposed to conceptual or physical models, simulation models enable numerical experimentation with alternative parametric assumptions for a given model design. Numerous design choices are made in model development that involve continuous or discrete representations of time and space. Simulation modeling approaches include system dynamics, discrete event simulation, agent-based modeling, and multi-method modeling. The model development process involves a shift from qualitative design to quantitative analysis upon implementation of a model in a computer program or software platform. Upon implementation, model analysis is performed through rigorous experimentation to test how model structure produces simulated patterns of behavior over time and space. Validation of a model through correspondence of simulated results with observed behavior facilitates its use as an analytical tool for evaluating strategies and policies that would alter system behavior.

Keywords: agent-based models, cellular automata, complex systems, computational laboratory, discrete-event simulations, dynamic systems, modeling, system dynamics

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Explanation

1. Introduction
2. Spatial Simulation
3. Design Choices
4. Model Analysis
5. Simulation Science

1. Introduction

Simulation modeling involves the use of computers to conduct virtual experimentation with alternative assumptions arising from “what if” questions about a dynamic problem of interest. By attempting to mimic the factual, simulation models may be used to explore the counterfactual (Morrison, 2015). In simulation modeling, computers provide a virtual world with which to experiment and thus gain insight into real-world problems and questions. This virtual experimentation is enabled by implementation of a model using a computer program or software platform to specify model structure and parameters that govern the boundary conditions of the model. Simulation is the execution of a sequence of model operations to produce output based on these model assumptions (Robinson, 2004; Gilbert and Troitzsch, 2005). While simulation models are generally used to study dynamic problems, with the goal of examining how system structure produces patterns of behavior for key variables over time, they may also be rendered spatially explicit to facilitate the study of such patterns over space as well as time.

The insight gained through the use of simulation modeling takes many forms. While prediction is, perhaps, the benefit most commonly associated with simulation models, researchers also employ simulation for other reasons, such as exploration, theory development, or even optimization of conditions to achieve desired outcomes. Some researchers use the virtual world of simulation modeling to improve understanding of complex social and environmental systems or to discover or formalize theories about the real world. As a scientific endeavor, simulation modeling is particularly useful for the study of complex systems, as the interconnections, feedback mechanisms, nonlinearities, and emergent behavior that characterize these systems are well suited for insights that arise from exploring various “what if”? questions over the course of successive simulation experiments.

2. Spatial Simulation

Spatial simulation modeling can be used to explore the emergence of spatial patterns over time (O’Sullivan and Perry, 2013). The grid-based cellular automata model, in which the state of each cell in a spatial array is updated at discrete time steps based on a particular set of rules, is perhaps the most widely-applied spatial simulation model (for more on cellular automata, see Cellular Automata. This spatial framework may be used to embed dynamic models in each grid cell as a spatial array of replicated models, each operating in parallel and interacting with neighboring models, such as through migration. These spatial simulation models can be used to model how the dynamics in one place can influence the dynamics in the surrounding areas. For example, Tobler (1970) demonstrated how differential equation models could be simulated in a spatially interconnected array for the case of urban population dynamics.

Spatially explicit simulation models may involve abstract or empirically-based GIS landscapes. GIS layers can be incorporated into simulation software platforms such as AnyLogic and NetLogo to enable spatially explicit simulation of model behavior. Vector layers can be used to locate agents, define transportation networks, and indicate regions over which individual information may be usefully aggregated. These representations correspond to an object-based (discrete) view of space. Raster layers can be used to define a grid akin to cellular automata in which model structures are embedded. These representations reflect a field-based (continuous) view of space. For example, a raster landscape was used to specify ash tree coverage in a spatial diffusion model of the invasive

Emerald Ash Borer (BenDor & Metcalf, 2006). Combining object-based and field-based representations, Westervelt and Hopkins (1999) simulated mobile objects within a dynamically changing grid-based landscape in a model of the Desert Tortoise foraging for vegetation in an area impacted by military training exercises.

BenDor and Kaza (2012) consider how different representations of space may be used to explore the possibilities for spatial dynamic simulation modeling. For example, replicated dynamic models can be spatially interconnected via a spatial network structure as well as a grid-based array. Although most spatial simulation models operate in 2-dimensional space, model dynamics may also be visualized in 3-dimensional space, as illustrated in Figure 1 for examples from the AnyLogic model library involving traffic flow at a roundabout and operations at a railyard, grain terminal, and passenger terminal.

Figure 1. Spatial simulation models of transportation in the AnyLogic software platform. Source: [AnyLogic](), with permission.

3. Design Choices

The development of a dynamic simulation model involves multiple design choices about model structure (Gilbert and Troitzsch, 2005). These choices include whether the model will be spatially explicit, and if so, how space will be represented and integrated into the dynamics of the model, as discussed in section 2. Another choice is whether to use deterministic or stochastic (probabilistic) model assumptions for parameter settings. Deterministic models create a singular trajectory of behavior for a given set of model parameters, whereas stochastic models produce a range of behavior. This choice thus has implications for the number and nature of simulation experiments to be conducted as part of model analysis, as discussed in section 4.

Just as continuous (raster) and discrete (vector) representations of space are fundamentally distinct in GIS models, a fundamental design choice in dynamic simulation modeling is whether to implement model structures using continuous or discrete representations of dynamic phenomena. Whereas continuous representations of dynamic systems date back to the invention of calculus, discrete representations have emerged in the computer age. Indeed, the very use of computers for numerical integration of continuous systems involves discretization in the form of the time step.

3.1. Continuous Representations

Continuous representations in simulation modeling entail numerical integration of differential equations, often to explore solutions beyond those that are analytically tractable. System dynamics is a method for modeling continuous systems using coupled ordinary differential equations that is distinguished by its visual representation of stock-flow structures and feedback mechanisms (Sterman, 2000; Ford, 2010). A stock is a state variable that integrates its net inflow (i.e., inflow minus outflow) to update its state at each time step. Changes in the level of the stock are thus governed by its flows, which are rates of change expressed in units of the stock over time.

In the iconography of system dynamics, the stock is represented using a box to symbolize a reservoir, whereas the flows are represented as pipelines with control valves that enter (inflows) or leave (outflows) the stock. In the example shown in Figure 2, the population stock is increased by inflows for birth and in-migration rates, and decreased by outflows for death and out-migration rates. As illustrated in Figure 2, parameter settings are adjustable using the slider bars to immediately see changes in population behavior that result from different settings for birth rates, life expectancy, and migration. Feedback mechanisms are either reinforcing (positive) feedback mechanisms that amplify change or balancing (negative) feedback mechanisms that counteract the direction of change. Two feedback loops are identified in Figure 2, with R indicating the reinforcing dynamics of reproduction and B indicating the balancing dynamics induced by deaths.

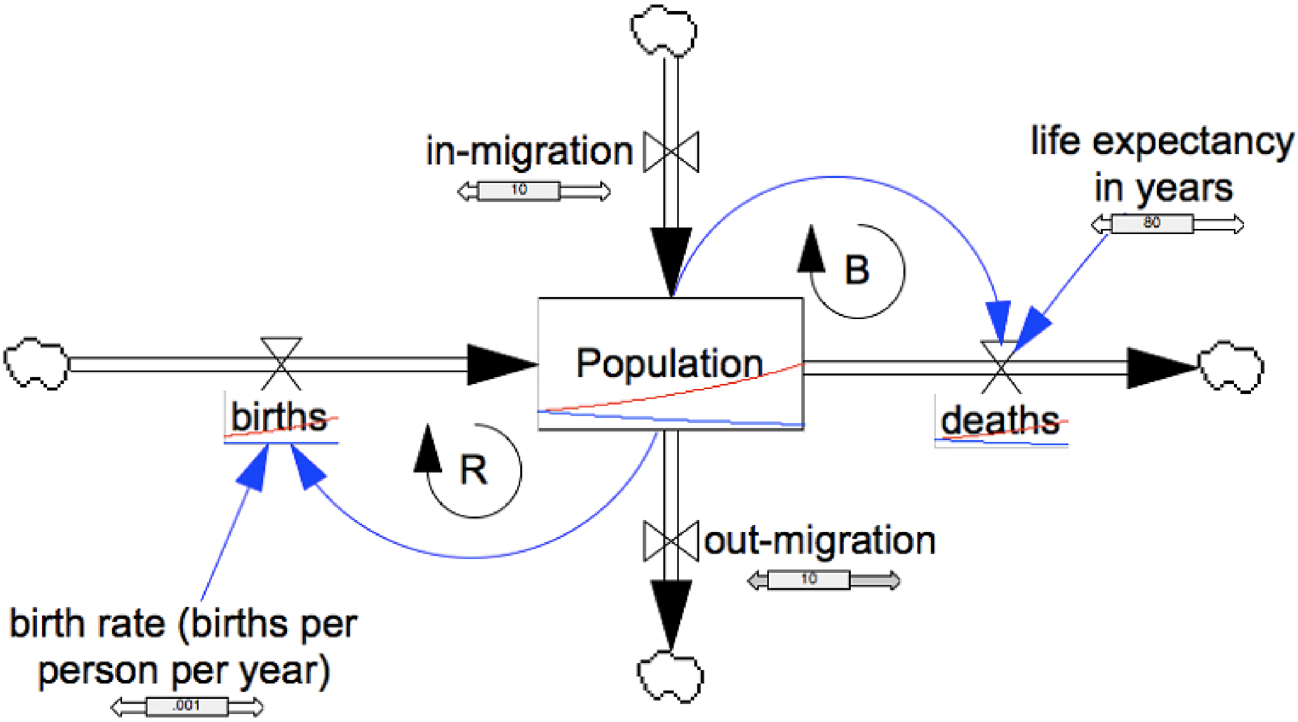

Figure 2. System dynamics simulation of population model using Vensim Synthesim to simulate output as parameters are adjusted with slider bars. Source: authors.

The capacity to replicate differential equation and system dynamics models in spatial arrays akin to cellular automata has enabled their use in simulating certain spatially-dependent dynamic processes, such as the coastal dynamics of sea-level rise (Ruth & Pieper, 1994), water levels in a drainage basin (Ford, 2010), population and migration dynamics in the Detroit region (Tobler, 1970), and the spread of invasive Emerald Ash Borer beetles among ash trees in suburban Chicago (BenDor & Metcalf, 2006).

3.2 Discrete Representations

Numerous approaches to simulation modeling involve discrete representations. Commonly used approaches include discrete event simulation, cellular automata, and agent-based modeling. Discrete event simulation, also known as process modeling, is a form of simulation modeling widely used in operations research to represent queuing behavior and other micro-level dynamics in contexts such as manufacturing plants, medical clinics, retail stores, and transportation terminals (Robinson, 2004). These models are often constructed using modular components to represent features such as buffers and switches. Rather than updating state variables at regular intervals defined by a time step, discrete event simulation models advance to the point in time when the next event is scheduled to occur.

Agent-based modeling entails the interaction of individual, discrete software entities known as agents. Agent behavior is encoded using algorithms at the individual level to define decision rules that control discrete transitions from one state to another. The earliest agent-based models of residential segregation (Schelling, 1971) reflect the tradition of cellular automata in simulating household agents in a grid-based spatial array. Indeed, agents are like cellular automata in that they involve interactions among autonomous entities that result in emergent aggregate behavior and threshold-based behavior. While agents and cellular automata often involve synchronous updates at each time step, they may also be designed to update their states asynchronously. But agents may be mobile, whereas cellular automata are spatially fixed. For instance, Westervelt and Hopkins (1999) model Desert Tortoise animals as individual agents that move and interact in a simulated landscape. Grimm and Railsback (2005) provide numerous examples of how dynamics of individual plants and animals are simulated in the ecological context. Agents may also be connected via static or dynamic social networks. The ability to create or destroy agents in the course of a simulation run provides a distinct contrast to population modeling in the tradition of system dynamics, in which stocks accumulate or deplete but never leave the system.

3.3. Multi-method Modeling

Multi-method approaches to simulation modeling draw from more than one modeling paradigm. This may include a portfolio of models using different approaches or integration of different approaches in a hybrid model. A hybrid model may include both continuous and discrete representations, allowing researchers to model processes that change gradually as well as abruptly. Hybrid models offer the flexibility to represent the structure of the system as appropriate for the scale at which it is modeled. An example of model hybridity would be to integrate system dynamics with agent-based approaches at different nested scales, allowing either the states of an agent's environment or within the agent itself to be governed by the feedback and stock-flow structures of system dynamics modeling (Swinerd & McNaught, 2012).

Figure 3 illustrates a schematic of hybrid modeling in which warehouse operations are modeled using discrete-event simulation, warehouses are networked as interdependent agents in a global supply chain, and global market dynamics are modeled using the stock-flow structures of system dynamics.

Figure 3. Schematic of a hybrid model using AnyLogic to represent warehouse operations and market dynamics in a globally networked supply chain. Source: AnyLogic, with

permission.

4. Model Analysis

Analysis of simulation models is essential to their use in advancing scientific knowledge (Rahmandad et al, 2015). However, because model analysis is undertaken in the later stages of the model development process, it is often neglected by novice modelers for the sake of expediency.

The modeling process is often viewed as an iterative cycle consisting of a sequence of steps taken to conceptualize, implement, and analyze the model to gain the desired insight (Sterman, 2000; Grimm and Railsback, 2005; Ford, 2010). The iterative nature of this process is critical, as the knowledge gained through various steps can – and should – be used to refine the assumptions outlined in previous steps. Although the recommended number and nature of these steps varies, the following stages of development are generally included:

1. Characterization of problem and research questions.
2. Development of dynamic hypotheses and conceptual models.
3. Implementation of model structure in the form of equations and algorithms appropriate to the design choices made.
4. Experimentation with the model to verify the structure and validate its behavior.
5. Analysis of alternative scenarios and how policies affect system behavior.

In this sequence, model implementation (step 3) marks the shift from qualitative to quantitative modeling, as parameters are specified along with the order of operations for the model. The first part of step 3 involves the selection of a simulation platform in which to encode model dynamics. Some user-friendly software platforms are indicated in the Additional Resources section, such as Stella and Vensim for system dynamics modeling, NetLogo for agent-based modeling, and AnyLogic for multi-method (discrete event, agent-based, and/or system dynamics) modeling. Successful completion of step 3 produces a simulation model with which to perform model analysis, as articulated in steps 4 and 5 of this process.

Model testing begins with verification to ensure that the simulation model is implemented as intended. This involves debugging, addressing errors, and performing boundary testing to see whether the logic of the model breaks down under extreme conditions, thereby delineating the range of conditions under which the logic of the model holds. Calibration of a model is performed by estimating parameter values so as to correspond with empirical observations. Validation is then undertaken to ensure that the simulation model is an appropriate representation of the real system. As with calibration, empirical observations are often used for model validation to determine how well simulated results correspond with empirically observed patterns of behavior. Data used for model validation, then, must be different from data used for model calibration.

Sensitivity testing is undertaken to understand the influence of parametric uncertainty on simulated output and identify which parameters have the greatest leverage in affecting model behavior. Threshold values may be identified as bifurcation points where a slight difference in the parameter setting produces a divergent pattern of behavior. Additional testing is needed for stochastic simulation to account for alternative random seeds, so emergent patterns are often averaged across a set of runs.

Monte Carlo methods for model analysis involve random sampling of parameter space to generate alternative realizations of a simulation experiment. This approach to sampling parameter space can reveal bifurcation or tipping points in which small changes in parameter settings induce qualitatively distinct patterns of behavior over time.

In some cases, optimization of model settings to achieve a desired outcome may be feasible and appropriate. Optimization is the process of determining an ideal selection of input values to satisfy the criterion of an objective function (e.g., minimizing cost, maximizing accessibility). If the system being modeled has a goal that can be defined as an objective function, then Monte Carlo analysis can reveal which parameter settings are optimal for achieving the goal. The parameter settings revealed through optimization are then associated with particular policy solutions or strategies.

By undertaking analysis to understand how model structure produces its behavior, model users are equipped to explore potential outcomes of alternative policy scenarios, simulating responses to various “what if?” questions. Therefore, in addition to its potential to advance science through simulation experiments, a simulation model can also confer practical utility as a decision support tool to inform policy, since simulation models can be used to explore the potential outcomes of different policies and practices that could be implemented to address a problem.

5. Simulation Science

Simulation modeling offers a means to advance scientific understanding of the complex, dynamic systems underlying the world’s most pressing problems. Unlike experiments in the real world, computational experiments conducted with simulation models may be replicated by others to allow for outside verification as well as extension to advance further research. Simulation science has also advanced in its capacity for representing model structures and dynamics using hybrid and multi-method modeling approaches that enable researchers to model systems that exhibit both continuous and discrete changes.

The capabilities of simulation modeling, and, consequently, its potential impact, are only increasing with improved computational capacity and flexibility of software programs to account for greater real-world dynamic complexity. In particular, simulation science has benefitted from advances in spatial dynamic modeling, as the integration of dynamic modeling with GIS landscapes offers the ability to simulate spatio-temporal patterns of complex systems with increasing ease. With this integration comes the ability to visualize behavior over time and space using geographic information science and technology.

Along with richer GIS landscapes for simulation are the prospects for improved model validation using Big Data. However, modelers must be selective in determining which data are appropriate for validating their models, since empirical data contain noise beyond what would be reasonably produced from a simplified model. Furthermore, different model structures and parameter settings may produce behavior that fits observational data equally well, known as the equifinality problem (O’Sullivan and Perry, 2013). This problem underscores the importance of simulation for the purpose of insight from experimentation rather than the search for a singular solution.

Modelers must be even more careful, then, to discern signal from noise in the great amount of Big Data now available. This word of caution, of course, is nothing new: a modeler's own wisdom and discernment are critical tools for using simulation models to improve their understanding of problems in the real world.

References

BenDor, T. K. and Kaza, N. (2012). A spatial theory of archetypes. System Dynamics Review, 28(2): 109-130.

BenDor, T. K. and Metcalf, S. S. (2006). The spatial dynamics of invasive species spread. System Dynamics Review, 22(1): 27-50.

Ford, A. (2010). Modeling the Environment, 2nd Edition. Washington: Island Press.

Gilbert, N. and Troitzsch, K. G. (2005). Simulation for the Social Scientist, 2nd Edition. Princeton: Princeton University Press.

Grimm, V. and Railsback, S. F. (2005). Individual-based Modeling and Ecology. Princeton: Princeton University Press.

Morrison, M. (2015). Reconstructing Reality: Models, Mathematics, and Simulations. Oxford: Oxford University Press.

O'Sullivan, D. and Perry, G. W. (2013). Spatial Simulation: Exploring Pattern and Process. Chichester: John Wiley & Sons, Ltd.

Rahmandad, H., Oliva, R. and Osgood, N. D., eds. (2015). Analytical Methods for Dynamic Modelers. Cambridge: MIT Press.

Robinson, S. (2004). Simulation: The Practice of Model Development and Use. Chichester: John Wiley & Sons, Ltd.

Ruth, M. and Pieper, F. (1994). Modeling spatial dynamics of sea-level rise in a coastal area. System Dynamics Review, 10(4): 375-389.

Schelling, T. C. (1971). Dynamic models of segregation. The Journal of Mathematical Sociology, 1: 143-186.

Sterman, J. D. (2000). Business Dynamics: Systems Thinking and Modeling for a Complex World. Boston: Irvin/McGraw-Hill.

Swinerd, C. and McNaught, K. R. (2012). Design classes for hybrid simulations involving agent-based and system dynamics models. Simulation Modelling Practice and Theory, 25: 118-133.

Tobler, W. R. (1970). A Computer Movie Simulating Urban Growth in the Detroit Region. Economic Geography 46: 234–240.

Westervelt, J. D. (1999). Modeling mobile objects in dynamic landscapes. International Journal of Geographical Information Science, 13(3): 191-208.