

Complex Systems Analysis using Space-Time Information Systems and Model Transition Sensitivity Analysis

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Abstract

Real-world systems are dynamic, complex and geographic, yet many mathematical modeling tools do not evaluate sensitivity of results to underlying assumptions, and GIS do not adequately represent time. This presentation describes two new approaches: Space-Time Information Systems (STIS), and Model Transition Sensitivity Analysis (MTSA). Current GIS are based on spatial data models that inadequately characterize the temporal dimension needed for effective representation of complex systems. They do not deal readily with space-time georeferencing nor space-time queries, and are best suited to “snapshots” of static systems. These deficiencies prompted many geographers to call for a “higher-dimensional GIS” (a STIS) to better represent space-time dynamics. When formulating models of complex systems, critical choices are made regarding model type and complexity. *Model type* is the mathematical approach employed, for example, a deterministic model versus a stochastic model. *Model complexity* is determined by the amount of abstraction and simplification employed during model construction. A growing body of work demonstrates that choice of model type and complexity has substantial impacts on simulation results and on model-based decisions. This paper briefly describes STIS and MTSA approaches that allow researchers to more effectively represent complex systems and to evaluate the sensitivity of their results to underlying assumptions.

1. Introduction

Jacquez (1996) and others describe a loose hierarchy for the modeling of complex systems, consisting of four steps or stages, cognitive models, exploratory data analysis, models of data, and models of process, each of which informs the others.

Cognitive and ontological models have to do with the mental representation of the underlying causal mechanisms that drive the relationships observed in a complex system. Typically, these are based on an understanding of the findings revealed by prior research, and by one’s own experience with similar systems. They guide exploratory data analysis, and form the basis on which more detailed data- and process-based models are constructed.

Exploratory Data Analysis (EDA) is founded on exploratory methods for quickly producing and visualizing simple summaries of data sets (Tukey 1977) that reveal relationships among variables and lead to insights that often cause one to refine the cognitive model. Insights from EDA can generate hypotheses that can be evaluated using inferential statistics and other data-based models. The objective of exploratory techniques is to explore and quantify relationships in order to increase the analyst’s knowledge of the complex system.

Models of Data include statistical tools such as ANOVA, regression and correlation, and are used to quantify relationships among variables, to test statistical hypotheses, and to identify factors that drive variability in the experimental system. These models require data of sufficient quality to estimate model coefficients (e.g. regression intercept), and sufficient knowledge to be able to identify dependent and independent variables, and their relevant parameters. Models of data are often used for interpolation and for prediction but do not of themselves convey information regarding underlying causal mechanisms.

Models of Process are used for prediction and the assessment of interventions. They require a detailed understanding of the mechanics of the system being studied, and incorporate this understanding directly into the model itself. Examples of process models in public health include infection transmission systems in which the population is structured into susceptible, infectious, and immune subgroups, and in which the model parameters describe mechanistic processes such as infection transmission from infectious to susceptible individuals (Koopman, Jacquez et al. 2001).

Complex systems analysis thus requires an understanding of the patterns present in natural systems as well as the ability to mathematically model those patterns. This paper is concerned with two of the above modeling steps: The cognitive and ontological representation of georeferenced data, and the construction of mathematical models of process to predict future behavior and to evaluate the impacts of alternative interventions on the modeled system. In practice these activities are founded on a variety of simplifying assumptions regarding ontology, representation, and model type. The question then arises as to whether the resulting models do an acceptable job of capturing relevant system behaviors, or whether the behaviors from the model are artifacts of the simplifying assumptions. With funding from NIEHS and NIAID, we are developing methods and software for evaluating the sensitivity of models of complex systems to underlying assumptions.

2. Space Time Information Systems

Background: Real world systems typically are geographic, dynamic and complex. Because of their ability to handle georeferenced data, Geographic Information Systems (GIS) often are used to store, manipulate and visualize information describing geographic systems. GIS have been criticized for their focus on static representations and for making little progress beyond the traditional map worldview (Goodchild, 2000), which is attributable to the inadequacy of the underlying ontological representation and data models that focus on spatial rather than space-time coordinate systems. Numerous data models have been proposed for representing dynamic systems, typically founded on data models that describe an object ID, a spatial coordinate, and a time value or time stamp. Yearsley and Worboys (1995), proposed a space time object model that integrates abstract spatial data types with a geometric layer to construct a higher-level topological data model, Raper and Livingstone (1993) used an object oriented approach to represent dynamic spatial processes as spatio-temporal aggregations of point objects, and Peuquet and Duan (1995) formulated an event-based spatio-temporal data model (ESTDM) that maintains spatio-temporal data as a sequence of temporal events associated with a spatial object (see Miller 2004 for a review of alternative data models).

Implementation: We have implemented a space time data model that treats time both as a coordinate as well as an attribute, and have derived a comprehensive suite of spatial, temporal, space-time and complex queries, as well as novel visualization techniques (Jacquez 2005). Collectively, these functionalities comprise a Space-Time Information System (STIS) technology that is ideally suited to the representation, visualization and simulation of complex, dynamic geographic systems. The STIS technology has the following advantages. First, it is designed to function within a distributed environment with different levels of access and data security. This assures confidentiality of sensitive data. Second, it maintains a local version of the data thereby assuring rapid queries

and responses, thus avoiding the long delays typical of web-based GIS. Third, it is built on true space-time data structures, enabling complex space-time queries not possible in conventional “spatial only” GIS. Fourth, it has open methods technology that allows researchers to develop and “plug-in” their own space-time analysis modules. Fifth, it incorporates statistical tests for space-time pattern such as univariate and bivariate local indicators of spatial autocorrelation. Sixth, it employs dynamic linked windows that enable both cartographic and statistical brushing. Finally, it displays animated “movies” for exploring how health outcomes (e.g. disease incidence, prevalence, morbidity and mortality) change through space and time.

The STIS architecture consists of several components: an event handler, data management, spatial data management, a methods component, and a cross-platform graphical interface. The system components have been written in C++, and include an open Python interface for method customization, as well as the ability to add methods using an external dynamic linked library (dll). The STIS architecture interfaces with SQL database servers over the internet or an intranet, and this interface can be extended and customized for other data schemas. It also reads dbase files (*.dbf) and shapefiles (a standard GIS format). The spatio-temporal analysis module is optimized for quick spatial and temporal indexing of data using a Hilbert R-tree, and calculates adjacency, spatial weights, and complex queries required for space-time statistics and modeling.

3. Model Transition Sensitivity Analysis

Characteristic	DC-type	SC-type	IEH-type
Assumes infinite population size	yes	no	no
Assumes homogeneity within compartments	yes	yes	no
Allows evaluation of study design and data analysis methods	no	partially	yes
Models events deterministically	usually	rarely	rarely
Models events stochastically	rarely	usually	usually
Ease of mathematical analysis	easiest	OK	hard
Solved numerically	yes	sometimes	no
Simulated for analysis	often	often	yes
Complexity of analytic results	simplest	OK	complex

Table 1. Characteristics of DC, SC and IEH models (from Koopman, Jacquez and Chick, 2001).

Background: With funding from NIAID we are developing methods and software for undertaking Model Transition Sensitivity Analysis that allows researchers, for the first time ever, to transit seamlessly from a deterministic model of a given system, to its stochastic counterpart, and on to its individual event history (IEH) representation. When formulating models, critical choices are made regarding model type and complexity. Model type is the mathematical approach used to represent a system, for example, an ordinary differential equation model versus a discrete event model; or a deterministic model versus a stochastic model. Model complexity is determined by the amount of abstraction and simplification employed during model construction. A growing body of work demonstrates that choice of model type and complexity has substantial impacts on simulation results and on public health decisions (Anderson, Ng et al. 1989; Anderson, Gupta et al. 1990; Blower, Anderson et al. 1990; Boily and Anderson 1991; Anderson, May et al. 1992; Garnett and Anderson 1993; Jacquez

and Simon 1993; Becker, Bahrapour et al. 1995; Blower and Blower 1995; Ghani and Swinton 1997; Koopman, Jacquez et al. 1997; Adams and Chick 1998; Aral, Hughes et al. 1999). Despite this, most analyses only assess sensitivity to a model's parameter values. Sensitivity to model type and complexity assumptions is difficult because of the lack of model transition sensitivity analysis (MTSA) software. In the absence of MTSA software it is almost impossible for decision makers to assess whether a proposed course of action is a good choice, or instead is highly sensitive to model type and complexity and is therefore an artifact of model selection (Koopman, Jacquez et al. 2001).

Implementation: We are developing simulation tools that support a variety of model types, provide a common user interface, and that provide seamless transition from one model type to another. We have accomplished this for three model types: Deterministic Compartmental (DC), Stochastic Compartmental (SC), and Individual Event History (IEH). The characteristics of these model types are defined in Table 1.

Deterministic Compartmental (DC) models use ordinary differential equations to describe change in compartment sizes over time. DC-type models treat a system as a series of internally homogeneous bins or compartments. Individual units (people, other animals, molecules...) flow between compartments when their state changes (disease state in an infectious disease model, chemical form in an isotope model, etc). For populations compartments correspond to population subgroups, such as those individuals with influenza, and states that have to do, for example, with risk behaviors and stages of infection. This model type does not consider discrete individuals or discrete events, and instead models populations as compartments and compartment sets. DC models can be solved numerically to find the number of individuals in each compartment at specified time points, and we treat time in DC models as continuous. All flows between compartments happen simultaneously. These flows may be constant, or they may be a function of the source compartment, the sink compartment, or any other compartment in the system. If the flows depend on compartment sizes, then they change when compartment population sizes change, and the system is non-linear. As time passes, the system recalculates all such flows based on the new population sizes in each compartment. If a flow between two compartments is small, and the time interval of observation is narrow, then fractions of the compartment population (possibly fractions of individuals) can flow. DC models thus assume the populations within compartments are infinitely divisible. The MTSA software employs a dynamic-time step, Runge-Kutta algorithm (Press, Teukolsky et al. 1992) to simulate the DC-type model. DC models provide an estimate of the mean (average) behavior of the modeled system, but assume individuals are infinitely divisible, and that state transitions are not discrete. These assumptions are not realistic, especially when compartment (sub-population) sizes are small, and hence DC models ignore the stochasticity that is the hallmark of almost all real-world systems.

Stochastic Compartmental (SC) models, like DC models, treat the system as a series of bins or compartments. These compartments can be identical to their DC model counterparts. But SC-type models differ in three significant ways. First, the modeled population is a finite population of individuals. This relaxes the DC assumption of an infinitely divisible population. Second, the flows between compartments are discrete (integer-based not reals as for DC models) representing whole numbers of individuals. Third, events in SC models are probabilistic and thus introduce stochastic variation. This fluctuation models the random outcomes that are observed in real systems, such as uncertainties in whether an infection event occurs when infected and susceptible individuals contact one another. The distributions of the random fluctuations in an SC model are well defined in terms of the parameters of the analogous DC-type model. Flows on arcs that link two compartments of a DC-type model are continuous with model-specific rates. Flows on analogous arcs of an SC model are discrete, and are conceptualized as a continuous time Markov chain (Bratley, Fox et al. 1987). The times between state changes,

or events, occur with an exponential distribution whose rate depends on the state of the system. The rates of state changes in an SC-type model are chosen to be equal to the rates of continuous flows of DC-type models. Because of the randomness in SC-type models, however, random variation above and below equilibrium levels will be observed. Benaim & Hirsch (1995) rigorously proved through mathematical argument that a DC-type model can be derived as a limiting case of an SC-type model as the size of the discrete-population grows arbitrarily large. This theoretically general result is the basis of our DC to SC transition.

Randomness in simulation outcomes entails additional care for estimating steady-state means such as the endemic prevalence of infectious diseases. In order to derive estimates of steady-state means we use methods from the LABATCH tool (Fishman and Yarberry 1997). Standard Markov chain simulation methodology is used to simulate the SC-models (Law and Kelton 2000) along with custom optimizations to improve the simulation performance for population models. SC models allow one to capture the stochasticity inherent in populations comprised of discrete individuals, and to derive probabilistic estimates and distributions for outcomes of interest such as cumulative density functions, compartment residence times and how compartment sizes change through time.

Individual Event History (IEH) models *sensu strictu* explicitly simulate individuals and their connections to other individuals. Each individual keeps track of its own history during a simulation, and this past history can influence its behavior. Individual event histories can be useful to study more characteristics of individuals and events than can be conveniently specified in a DC or SC model. However, full-blown individual or agent-based models are simulations that lack much, if any, of a theoretical basis. In practice this makes it impossible to clearly and definitively specify the individual-based model that corresponds to a given DC or SC model, and hence to characterize the relevant assumptions. In our algorithms we therefore strike a middle ground that maintains the well-developed theory behind SC models, but allows us to report the event histories for individuals represented in the SC model. MTSA's IEH model operates by uniquely identifying all individuals in the SC models, and then recording all state transitions, aging and flow events that occur to that individual during the course of the simulation. This, in effect, creates "diaries" for each individual in the modeled population, and hence the individual event histories can be used in model validation by comparison to individual-based data that has been observed.

Time Representation: Because it can have a substantial impact on results, handling of time is critical in simulation studies. Our approach has been designed to provide the most realism, and SC- and IEH-type models handle time differently than DC-type models. As in a DC model, the system calculates the flow rate from each compartment, but these numbers are interpreted differently. Instead of simultaneous movement from all compartments, the SC and IEH models move one individual from one compartment at a time. This chooses one flow at random from all possible flows, with the probability of picking a flow proportional to its size. Stochastic model simulations are event-based, where an event is defined as a single individual changing compartments (for SC) or attributes (for IEH). Time in the model is incremented with each flow of one individual. If the individual is part of a large flow, the time step is short. If the individual is part of a smaller flow, the time step is comparatively larger. Time is thus updated discretely with time steps of varying duration. The time increment is drawn from an exponential distribution with a mean equal to the reciprocal of the chosen rate. This means that when a large rate, R , is chosen at random (which will happen more often because of weighting), time will advance by $1/R$ on average, which will be a small value. So flows with large rates will be chosen most often, but time will advance least when they are. This achieves the effect we desire: on average, common events occur more often.

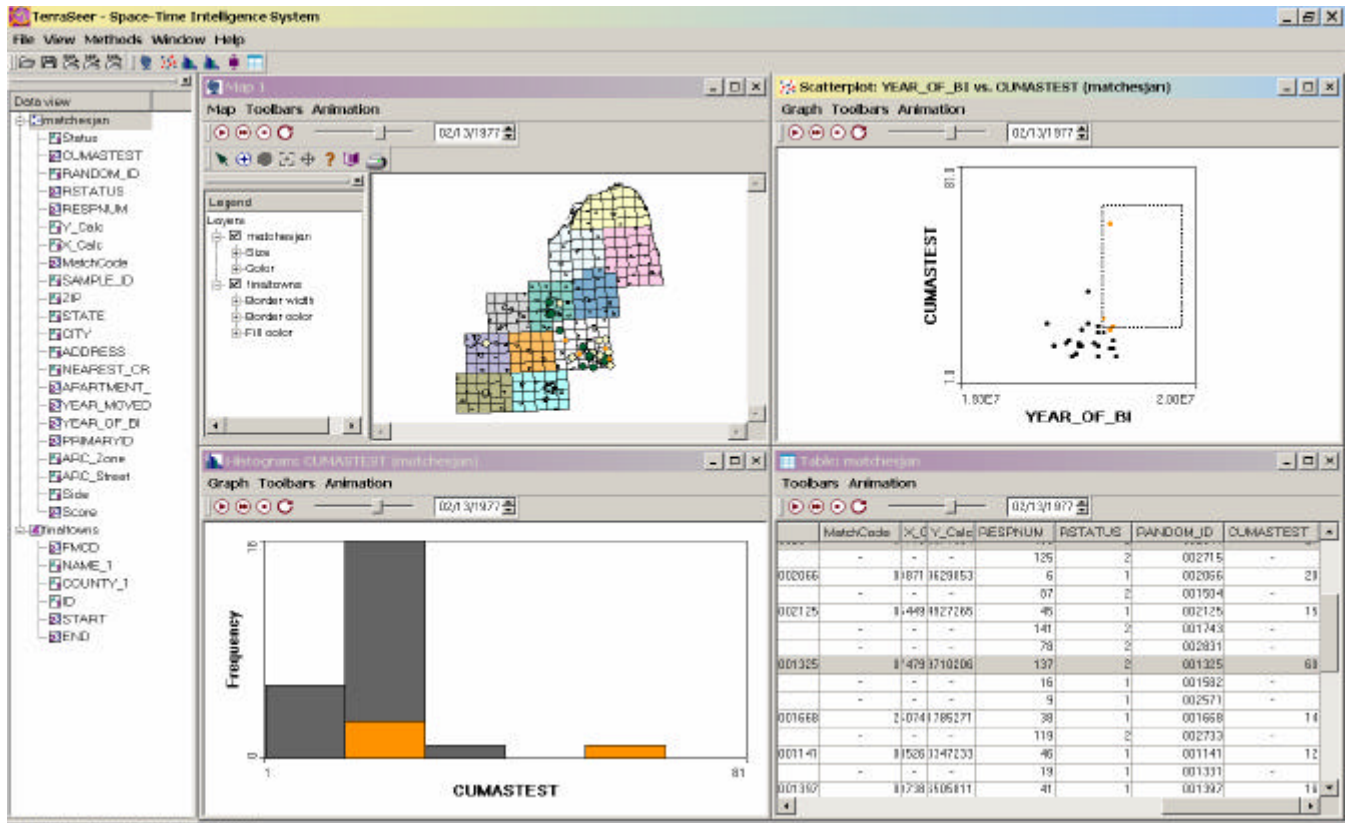


Figure 1: The STIS user interface. User's may temporally link map and statistical views to be synchronous during animation (shown is 1977). The user has selected young individuals with high cumulative arsenic (box in upper right window). Selected points are highlighted in the map, table and histogram views.

4. Results

STIS: Although still in development, STIS has been successfully deployed under NCI grant R01 CA92669 that created a STIS for the National Atlas of Cancer Mortality (<http://www.terraser.com/atlasviewer.html>). In addition, The University of Michigan (J. Nriagu PI), also with funding from NCI, is using STIS in a study of bladder cancer and exposure to arsenic in drinking water in southeastern Michigan. In that project the STIS is used to model water distribution systems to represent changes in spatial support since the 1920's; to model residence and occupational history of 800 cases and controls using geospatial lifelines, and to ultimately to estimate individual-level historical exposure to arsenic (Meliker 2005), as shown in Figure 1. The uncertainty attached to the space-time prediction of arsenic concentrations in groundwater will be assessed using geostatistics (see Goovaerts et al., 2004), and propagated through the exposure model using Monte-Carlo simulation, leading to an individual model of uncertainty for arsenic exposure.

In collaboration with Jim Koopman at The University of Michigan, we are using the MTSA software to evaluate alternative infection control approaches for Nontypeable *Haemophilus influenzae* (NTHi), a leading cause of childhood ear and sinus infections that can cause bacterial pneumonia. While not lethal, ear infections cost the U.S. health care system an estimated \$3.8 billion per year, and although *H. influenzae* is becoming increasingly resistant to antibiotics, vaccination is effective against the typeable *H. influenzae* strains. Developing a good NTHi immunization program depends on a clear understanding of NTHi transmission. By progressively relaxing the assumptions implicit in different modeling approaches, model transition sensitivity analysis allows us to

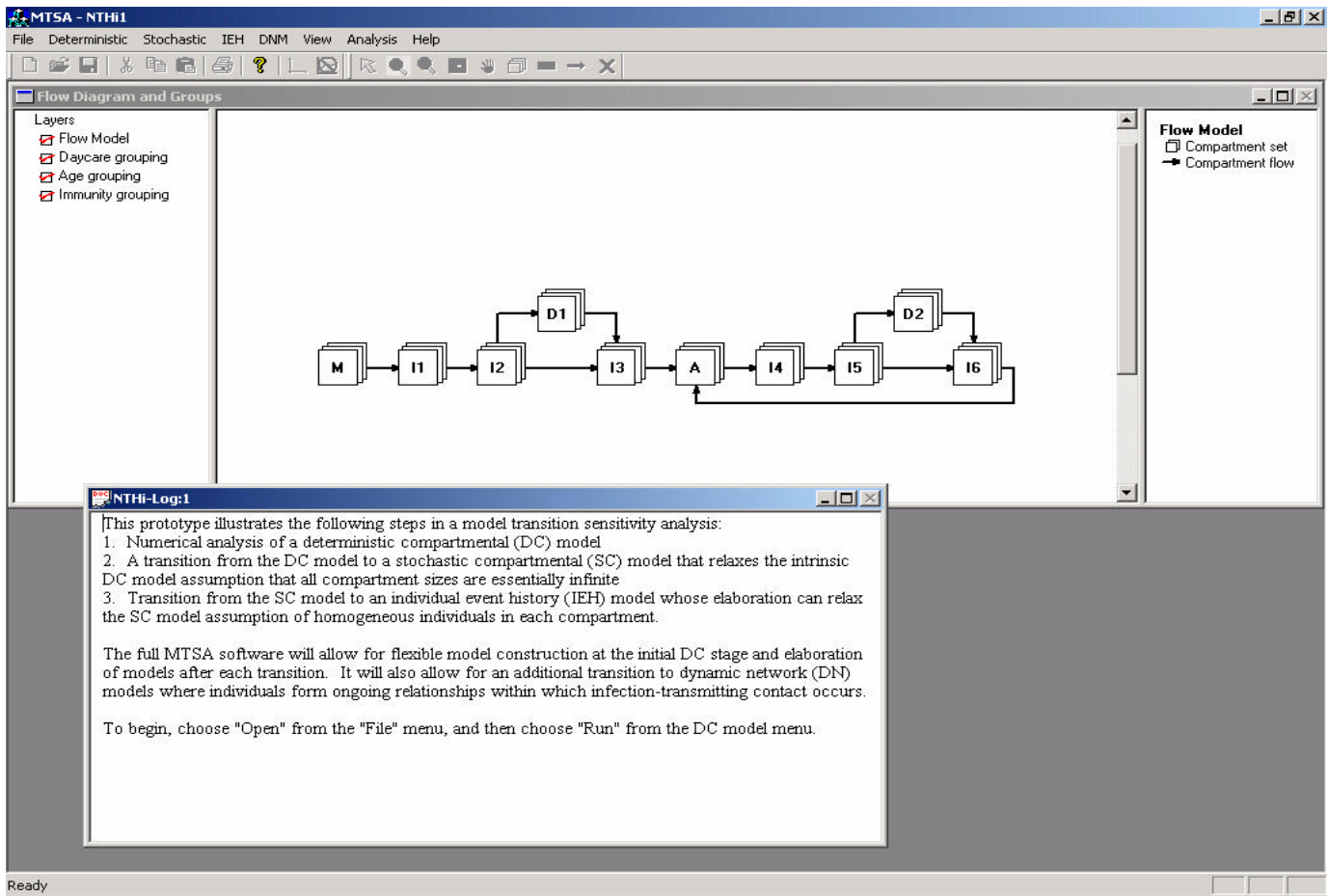


Figure 2. Main Form of MTSA Workbench.

identify model behaviors that are artifacts of model type. Upon invoking MTSA-NTHi the program's Main Form appears (Figure 2), consisting of a view of the flow diagram and groups at the top, and a log file at the bottom. This model is complex and has many dimensions that cannot be effectively represented in a single view. The "flow diagram and groups" view allows the user to rapidly interrogate and visualize model complexity.

The compartment sets labeled "M", "I1" and so on are different states that differ only in certain group characteristics, and hence they are "sets" of compartments. In this case we are modeling differences in infection and immunity status. "M" represents susceptible individuals with maternal immunity inherited from their mother's immune system. All births enter this compartment set. "A" represents individuals with acquired immunity to NTHi, gained by prior infection. I1, I2, I3, I4, I5 and I6 are the stages of infection for which individuals are infected but asymptomatic. D1 and D2 are the stages of infection that show symptoms of ear infection. Because NTHi infections can be asymptomatic, D1 and D2 can be bypassed in the flow model. Death does not result from NTHi infection, but it can occur at any stage in the flow diagram. For simplicity, this diagram omits birth and death flows.

In practice, many infection transmission systems are defined on local populations of a few thousand or even a few hundred individuals. Schools and daycare centers, for example, often have a few dozen to a few hundred students. Deterministic models assume individuals are infinitely divisible and that inter-compartment flows can be comprised of fractions of individuals. In practice infection events (e.g. becoming infected) involve a change in state of entire individuals, inter-compartment flows are better represented as whole numbers, and a stochastic

model that treats individuals as integer numbers is appropriate. The transition from a DC to an SC-type model is accomplished by selecting “Deterministic” on the Main Menu and “Transit to SC”. This causes the deterministic model to be translated into its stochastic counterpart as the above assumptions are relaxed. Graphs of population size through time can differ dramatically between DC and SC model types (Figure 3).

5. Conclusions

The goal of modeling is to formulate models that capture relevant aspects of system behavior while maintaining simplicity and ease of understanding. This is accomplished via abstraction and simplification.

Abstraction: Reality is highly complex and this complexity is made tractable by abstracting reality to represent important components within a representation (e.g. space-time data model) or mathematical form (the model type). Because they are abstractions, all models are “wrong” since they do not fully represent reality and thus cannot capture all behaviors of the modeled system (Koopman, Jacquez and Chick 2001). As abstractions models are most useful when they capture aspects of a system's structure and behavior deemed relevant to a specific problem.

Simplification of complex reality is required in order to formulate understandable representations and mathematical models. Hence there is a dynamic and a tension between simplification and the ability of representations and models to adequately characterize system behaviors.

Assumptions: Simplification is accomplished by making restrictive assumptions, and many such assumptions are intrinsic to the chosen ontology and model type. Thus one of the most important problems in modeling is to determine the sensitivity of model results, and of decisions based on those results, to assumptions of representation and model type. How can we determine whether an abstraction is appropriate, and how do we know when reality is oversimplified? These two issues underlie all models of complex systems, and are the fundamental questions answered by STIS and MTSA.

When evaluating complex systems simplifying assumptions must be made to make the modeling problem tractable. But when are such assumptions too simplistic, and when are they useful? One thus needs to determine the tradeoffs between abstraction and simplification, and realism and complexity. STIS addresses the profoundly simplistic assumptions implicit in most GIS models of – that complex geographic systems can be effectively characterized by a static representation. MTSA addresses two arenas of simplifying assumptions made in the

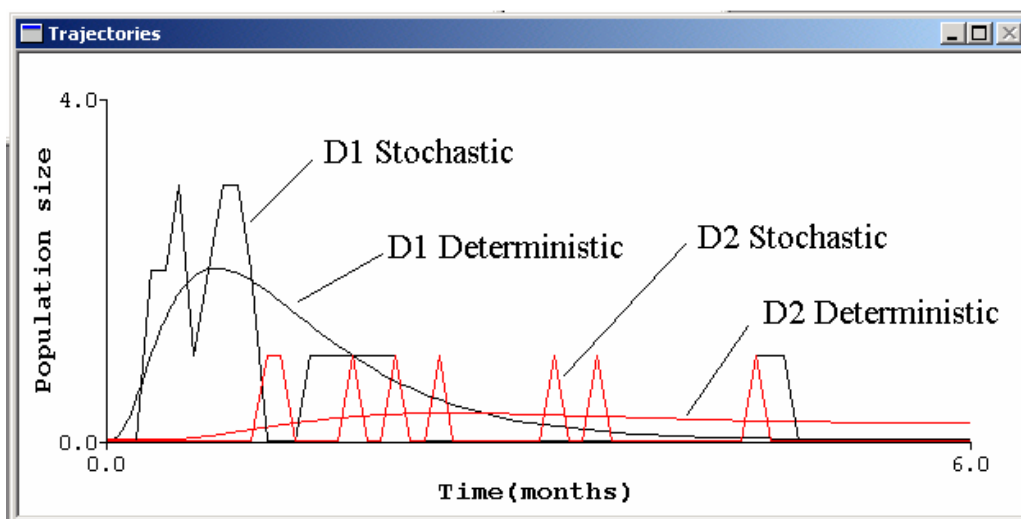


Figure 3. Stochastic and deterministic population trajectories for individuals symptomatic for otitis.

construction of mathematical models of complex systems – that of model type, and of model complexity. Together, STIS and MTSA are expected to be important tools for analyzing complex systems. The importance of evaluating sensitivity of results and decisions to assumptions of approach, whether these are representational, statistical or model-based, cannot be minimized.

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