RESEARCH ARTICLE

Modeling Complex Systems Macroscopically: Case/Agent-Based Modeling, Synergetics, and the Continuity Equation

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Recently, the continuity equation (also known as the advection equation) has been used to study stability properties of dynamical systems, where a linear transfer operator approach was used to examine the stability of a nonlinear equation both in continuous and discrete time (Vaidya and Mehta, IEEE Trans Autom Control 2008, 53, 307–323; Rajaram et al., J Math Anal Appl 2010, 368, 144–156). Our study, which conducts a series of simulations on residential patterns, demonstrates that this usage of the continuity equation can advance Haken's synergetic approach to modeling certain types of complex, self-organizing social systems macroscopically. The key to this advancement comes from employing a case-based approach that (1) treats complex systems as a set of cases and (2) treats cases as dynamical vsystems which, at the microscopic level, can be conceptualized as k dimensional row vectors; and, at the macroscopic level, as vectors with magnitude and direction, which can be modeled as population densities. Our case-based employment of the continuity equation has four benefits for agent-based and case-based modeling and, more broadly, the social scientific study of complex systems where transport or spatial mobility issues are of interest: it (1) links microscopic (agent-based) and macroscopic (structural) modeling; (2) transforms the dynamics of highly nonlinear vector fields into the linear motion of densities; (3) allows predictions to be made about future states of a complex system; and (4) mathematically formalizes the structural dynamics of these types of complex social systems. *Complexity 000: 00–00, 2012*

Key Words: continuity equation; macroscopic modeling; synergetics; case-based modeling; agent-based modeling; complex social systems

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1. INTRODUCTION

This article uses the continuity equation in a novel way to extend Haken's [1] synergetic approach to modeling complex social systems macroscopically, where transport or spatial mobility issues are of interest (e.g., residential mobility, traffic patterns, swarm behavior, groups/collective

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behavior, population densities). Our novel usage of the continuity equation is based on our unique approach to case-based modeling, which (1) treats complex systems as a set of cases and (2) conceptualizes cases as individual dynamic entities, which, at the microscopic level, are defined as k dimensional row vectors and, at the macroscopic level, as vectors with magnitude and direction, which, using the continuity equation, we model as population densities.

Our interest in the continuity equation (also known as the advection equation) is based on recent research where a linear transfer operator approach was used to examine the stability of a nonlinear equation both in continuous and discrete time [2, 3]. The main idea is that while the motion of individual cases (their trajectories) can be highly nonlinear, the motion of an ensemble of such trajectories is governed by a linear transfer operator, namely, the Perron-Frobenius operator. We see such an approach as directly relevant to synergetics.

Synergetics concerns itself with complex (nonequilibrium thermodynamic) systems that can "form spatial, temporal or functional structures by means of self-organization" [1]. Key to a self-organizing system is the emergence of order parameters, as opposed to control parameters. In a synergetic system, control parameters can be conceptualized as microlevel interactions and rules governing behavior, which can be grouped into one of two types: internal or external. In an agent-based or case-based model, for example, internal control parameters can be the microscopic rules governing the interactive transport of agents. In contrast, order parameters are macroscopic controls (which, sociologically speaking, can be thought of as social structure). In general, these controls are dimensionally "low dynamic." These order parameters (self-organizing, emergent social structures) are key to synergetics (and to our novel usage of the continuity equation) because their "low dynamics" allow them to be modeled macroscopically and, more specifically for our purposes, conceptualized formally as densities: despite the complexity, nonlinearity, or diversity of the microscopic (or mesoscopic) behavior of a self-organizing system's agents, at the macroscopic level these behaviors and their coordination can be modeled as population (probability) densities via the continuity equation.

Our novel usage of the continuity equation is directly connected to our work in agent-based and case-based modeling. While readers will be familiar with the former, the latter is a new area of study, so we will review it quickly. Case-based modeling (although traditionally not computational) is an established technique in the social sciences, used for conducting in-depth, idiographic, comparative analyses of cases and their variable-based configurations [4]. Only recently, however (as in the last few years) researchers have begun to explore its potential for modeling complex systems, particularly with large databases and as a computational technique [5–8]. The premise for this new line of inquiry, expressed by Byrne [5], is that cases are the methodological equivalent of complex systems.

Despite the differences between agent-based and case-based modeling, they both struggle with similar limitations, which the continuity equation, grounded in our case-based approach, can address. First, it provides a way to link micro-level and macro-level behaviors, as well as link agency (e.g., agent-based behavior) and structure (e.g., population densities). To connect microscopic rules to macroscopic patterns, the continuity equation allows the control parameters of a case-based or agent-based model to evolve across time/space to discover their macroscopic order parameters, which manifest themselves as transient motion of densities. Discovering the motion of densities leads to the second utility of the continuity equation: it transforms the dynamics of complex, nonlinear, and diverse vector fields into the linear motion of densities. Third, as a differential equation, it allows predictions to be made about future states of a complex system. Finally, it mathematically formalizes the structural dynamics of complex social systems where transport or spatial mobility issues are of interest, which is difficult in the social sciences to do.

To demonstrate the utility of our approach, our article is organized as follows. First, given the general familiarity of agent-based modeling, we provide a quick overview of case-based modeling by reviewing the SACS Toolkit, a new case-based modeling method that we developed. In terms of the continuity equation, the SACS Toolkit is important because it (a) conceptualizes complex systems as a set of cases and (b) treats this set of cases as a matrix of k dimensional vectors (cases) which, (c) at the macroscopic level, can be given magnitude and direction and modeled as population densities. Second, with a basic understanding of the SACS Toolkit and its case-based modeling approach established, we review the continuity equation, focusing on how a matrix of k dimensional vectors (be they cases or agents) can be converted into a vector field f with magnitude and direction, allowing for the transformation of nonlinear, complex, diverse case-based vector fields into population densities. Third, we apply our usage of the continuity equation to an example from our recent research on residential mobility patterns, conducting a series of simulations. Our focus on residential migration patterns was chosen because it is an example of a synergetic system where a complex, nonlinear microscopic vector field of diverse agents (each with its own magnitude and direction) self-organizes into an ordered and, scale-wise, spatially large complex system [6].

2. CASE-BASED MODELING AND THE SACS TOOLKIT: A MATHEMATICAL OUTLINE

Researchers in the social sciences currently employ a variety of mathematical/computational models for studying complex systems. Despite the diversity of these models, the majority can be grouped into one of four types: agent

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(rule-based) modeling, dynamical (equation-based) modeling, network (structural) modeling, and statistical (aggregate-based) modeling. Case-based modeling constitutes a fifth type [6, 9]. The premise for this new line of inquiry, expressed by [5], is that cases are the methodological equivalent of complex systems. One such example of a case-based model designed for studying complex systems, which we review here, is the SACS Toolkit [9].

2.1. Complex Systems as *k* Dimensional Vectors/Cases

The SACS Toolkit is a case-based, mixed-method, system-clustering, data-compressing, theoretically driven toolkit for modeling complex social systems. Its vector-based approach to modeling [10] is defined as follows:

1. The SACS Toolkit is a variation on Byrne's [5] general premise regarding the link between cases and complex systems.
2. For the SACS Toolkit, case-based modeling is the study of a complex system S as a set of cases c_i such that:

$$S = \{c_i : c_i \text{ is a case relevant to the system under study.} \tag{1}$$

3. At minimum, S is composed of one case c_i.
4. We denote the number of cases being studied by n.
5. Each case c_i in S is a k dimensional row vector $c_i = [x_{i1}, \ldots, x_{ik}]$, where each x_{ij} represents a measurement on one of the variables being used to model a complex system.
6. The variables used to model a complex social system are one of two types: social practices P_i and environmental forces E_i.
7. Social practices P_i are the social system's variables, including social, cultural, economic, political, and psychological factors. The set of social practices is called the *web of social practices* W_s, where

$$W_s = \{P_i : P_i \text{ is a social practice relevant to the system of study}\}. \tag{2}$$

8. As a set of social practices W_s, a complex system S is externally impacted by a set of environmental forces E_s, which consists of individual environmental forces denoted by E_i. We write the set of all environmental forces as follows:

$$E_s = \{E_i : E_i \text{ is an environmental force relevant to the system of study}\}. \tag{3}$$

9. A complex system S (and its set of cases) self-organizes around and emerges out of the coupling of social practices P_i and environmental forces E_i.
10. Because S consists of n cases $\{c_i\}_{i=1}^{n}$, and each case c_i has a vector configuration of k dimensions, it is natural to represent S, at least initially and at its most basic, in the form of a data matrix D as follows:

$$D = \begin{bmatrix} c_1 \\ \vdots \\ c_n \end{bmatrix} = \begin{bmatrix} x_{11} & \ldots & x_{1k} \\ \vdots & \ddots & \vdots \\ x_{n1} & \ldots & x_{nk} \end{bmatrix}. \tag{4}$$

11. In the notation above, the n rows in D represent the set of cases $\{c_i\}$ in S, and the k columns represent the measurements on some finite partition $\cup_{i=1}^{p} O_i$ of W_s and E_s that couple to form the vectors for each c_i.
12. Putting the above together, we can summarize D as shown in (4), where each $c_i \in D$ is a case-based k dimensional row vector $c_i = [x_{i1}, \ldots, x_{ik}]$ composed of a set of measurements on W_s and E_s; and, the k-dimensions of each c_i in S can be thought of as the vertices of a graph, with vertices being nonempty elements of any finite partition of W_s or E_s.

3. COMPLEX SYSTEMS ACROSS TIME/SPACE

1. While the above definition is discrete, cases c_i (like agents in agent-based modeling) ultimately are not static; they are dynamic and evolving. For the SACS Toolkit, therefore, cases c_i are ultimately treated as discrete dynamical systems $c_i(j)$, where j denotes the time instant t_j.
2. If cases c_i change across time/space, so too must their vector configurations $c_i = [x_{i1}, \ldots, x_{ik}]$; that is, their measurements on W_s or E_s in D. As such, D is composed of a series of $c_i(j)$, one for each discrete moment in time/space t_j, on which a set of measurements are taken to construct a particular model of S.
3. If cases are discrete dynamical systems $c_i(j)$ (continuous time dynamical systems represented as $c_i(t)$ with time t being continuous), it therefore follows that, as a final definition, a complex system S is a set of cases $\{c_i\}$, with each case c_i constituting one of its possible ways of practice across time/space, based on the coupling of W_s and E_s.

4. MODELING CASES/AGENTS MACROSCOPICALLY

Because the SACS Toolkit is a data compression (as opposed to data reduction) technique, the cases/agents within a complex system can be studied at multiple levels of analysis, from the microscopic to the macroscopic, as well as at the intersection of these different levels of scale. At the macroscopic level, the focus is on the entire complex system (as a set of interacting cases), particularly its movement across time/space, as in the case of the continuity equation. Switching to the macroscopic level, however, requires the concept of cases as vectors to be developed.

4.1. Cases as Euclidean Vectors

Applying the continuity equation, the SACS Toolkit reduces the set of cases/agents in a complex system to a Euclidean vector field, which we can write as follows:

$$c_i \approx f(x). \tag{5}$$

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Following this equation, each case in a complex system is mapped to a vector $f(x)$ placed at a position x. Assignment of magnitude and direction to this vector field is based on empirically grounded, case-based information, often simulated in the form of some agent-based model, learned earlier (as we explained in the Introduction section) by allowing the macroscopic patterns of the model to emerge. In so doing, these emergent, self-organizing patterns can be transformed (in terms of order parameters) into population densities, with appropriate assignment of vector field $f(x)$.

Because macroscopic modeling (which, in this case, is done using the continuity equation) is a consequence of what was learned by studying a microscopic (e.g., agent-based or case-based) model and its microscopic control parameters, we see it as assisting agent-based and case-based modeling. It picks up where they leave off, so to speak, allowing us to formalize, as order parameters, its structural dynamics in mathematical terms. We turn, now, to a more formal review of the continuity equation.

5. THE CONTINUITY EQUATION

The continuity equation has been used extensively in fluid mechanics and electromagnetism to model the transport of physical quantities such as mass and charge, respectively [11, 12]. The key aspect of the continuity equation, particularly for social scientists to understand, is that it models the transport of a physical quantity (which could be anything, including people, social groups, traffic patterns, swarm behaviors, populations, etc) according to a given vector field f in addition to conserving the physical quantity itself. The dynamical state of the continuity equation is typically a density function. The density function ρ is nothing but the physical quantity per unit area in two dimensions. Recently, the continuity equation (also known as the advection equation) has been used to study stability properties of dynamical systems, where a linear transfer operator approach was used to study the stability of a nonlinear equation both in continuous and discrete time [2, 3].

6. THE CONTINUITY EQUATION AS A MODEL FOR RESIDENTIAL MOBILITY

Given its complexity, particularly for social scientists, we can only provide here a very quick overview of the continuity equation. For those not familiar with this equation, see [2, 3]. The continuity equation is as follows:

$$\rho_t + \nabla \cdot (f\rho) = 0; \quad \rho|_{\Gamma_i} = 0; \rho(x, y, 0) = \rho_0(x, y), \qquad (6)$$

where $\rho(x, y, t)$ is the population density as a function of space and time variables; and, $(x, y) \in \Omega$, $t \in [0, \infty)$, $\Gamma_i = \{x \in \partial\Omega : f \cdot \eta < 0\}$ is the inflow portion of the boundary $\partial\Omega$, with η being the outward unit normal at every point on the boundary $x \in \partial\Omega$. The initial population density is given by $\rho_0(x)$, and hence by the conservation property of population mentioned above, we have the following where P_0 refers to the initial population:

$$P(t) = \iint_\Omega \rho(x, y, t)dxdy = \iint_\Omega \rho_0(x, y)dxdy = P_0. \qquad (7)$$

The solution of (6) can be written using the Perron-Frobenius linear transfer operator $\mathbb{P}_t : L^1(\Omega) \rightarrow L^1(\Omega)$, defined as follows:

$$\mathbb{P}_t \rho = \rho(\phi_{-t}(x)) \left| \frac{d\phi_{-t}(x)}{dx} \right|, \qquad (8)$$

where $\phi_t(x)$ denotes the flow map for $\dot{x} = f(x)$ starting at the point $x \in \mathbb{R}^2$, and $|\cdot|$ denotes the determinant of a matrix. For more details on the Perron-Frobenius operator, we refer the reader to [13].

7. APPLYING THE CONTINUITY EQUATION TO RESIDENTIAL MOBILITY

We recently completed a study on residential mobility and its impact on community-level health [6]. For our study, we were interested in the social phenomenon in the United States known as sprawl. In complexity science terms, sprawl is a series of microscopic behaviors engaged in by a network of individual agents. More concretely, it is the unplanned out-migration (flow) of affluent populations into the suburban and semi-rural tiers surrounding an urban area. The unplanned nature of sprawl comes from the fact that, like many synergetic systems, no single force or agent is steering it. Instead, the complex system is evolving, self-organizing, and emerging on its own, the result of a large number of adaptive, self-focused agents, across different communities, interested in upward social mobility.

As sprawl evolves, it creates a geographical network of segregation and exclusion where communities become, in many ways, relative islands in terms of resource usage, politics, wellbeing, and so on, with movement among communities being largely automobile dependent. A significant, macroscopic consequence of this segregation is that communities tend to be divided into rich, middle and poor, with the poor communities falling into what Bowels et al. [14] call a poverty trap: a self-reinforcing situation of persistent and intractable poverty. In short, sprawl is a complex systems problem.

To examine this issue, we built a simple agent-based model, based on an in-depth empirical inquiry of a Midwestern County in the United States. The model we built was called Summit Sim. (To run the model or download its code, visit `http://www.personal.kent.edu/~mdball/pareto_schelling_mobility.htm`.) In our two-dimensional model are three populations: rich, middle, and poor. Sprawling movement in Summit-Sim is based on three rules: (a) rich agents seek to live near rich agents; (b) middle-class agents seek to live near rich agents; if they cannot, they seek to live near other middle-class agents; if they find themselves in a

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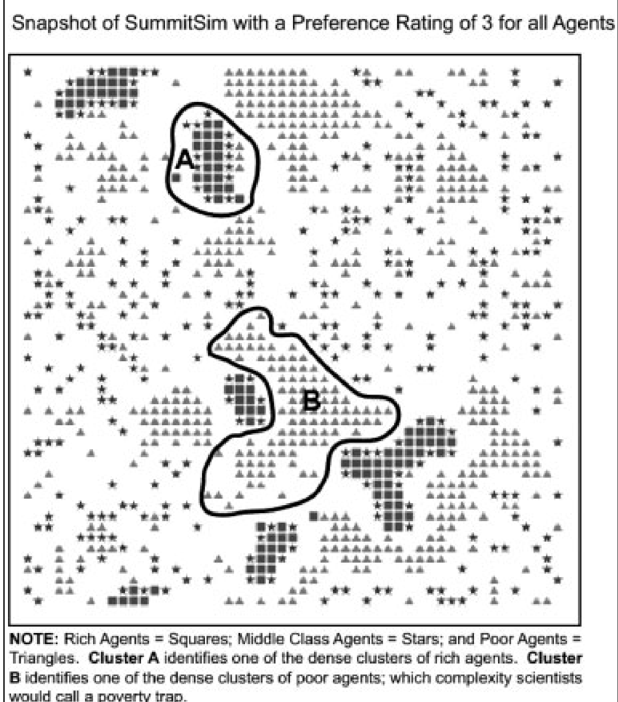
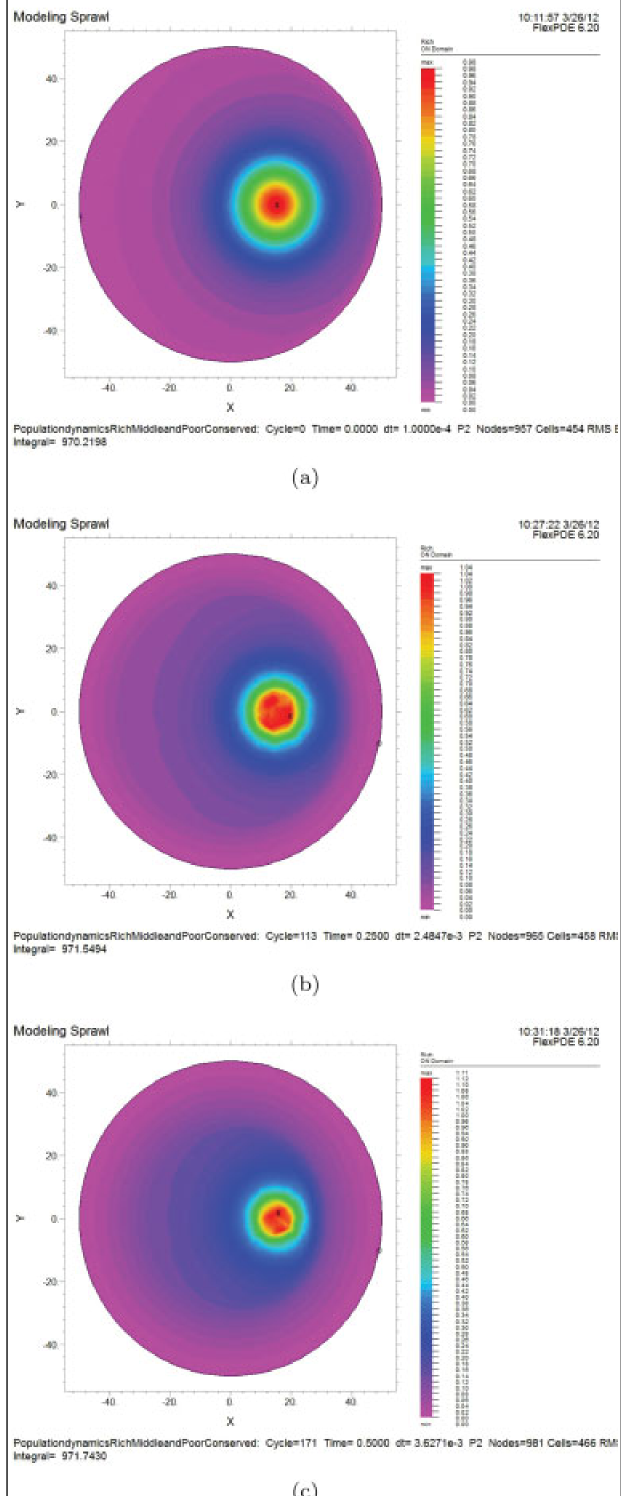
FIGURE 1



Steady state distribution of rich, middle class, and poor agents using Summit-Sim.

FIGURE 2



Contour plots of rich density at the initial, intermediate, and final time instants for scenario 1.

neighborhood with four or more middle-agents, they stay; and (c) poor agents seek to live near middle-class agents; if they cannot, they stay where they are. The mobility of rich, middle class, and poor agents was programmed in decreasing order. In addition, a preference degree that is, the number of rich agents that are required to satisfy the rich, etc., was programmed. As shown in Figure 1, it was seen in Summit-Sim that regardless of the initial distribution of agents, as long as the preference degree was kept below a certain threshold spatial segregation and clustering resulted.

The question, however, was why did this macroscopic order emerge? In other words, was it possible to mathematically state how the microscopic rules governing the behavior of these three coupled populations resulted in the macroscopic pattern we found? It was at this point that, given the utility of synergetics for dealing with such types of systems, we turned to the possibility of order parameters and the continuity equation. For our macroscopic model, social mobility was formally defined as modeling the evolution of rich, middle class, and poor population densities in a given two-dimensional domain $\Omega \subset \mathbb{R}^2$. For our model, we made the following assumptions:

1. We modeled the evolution of a population density ρ rather than an actual population P because the former lends itself

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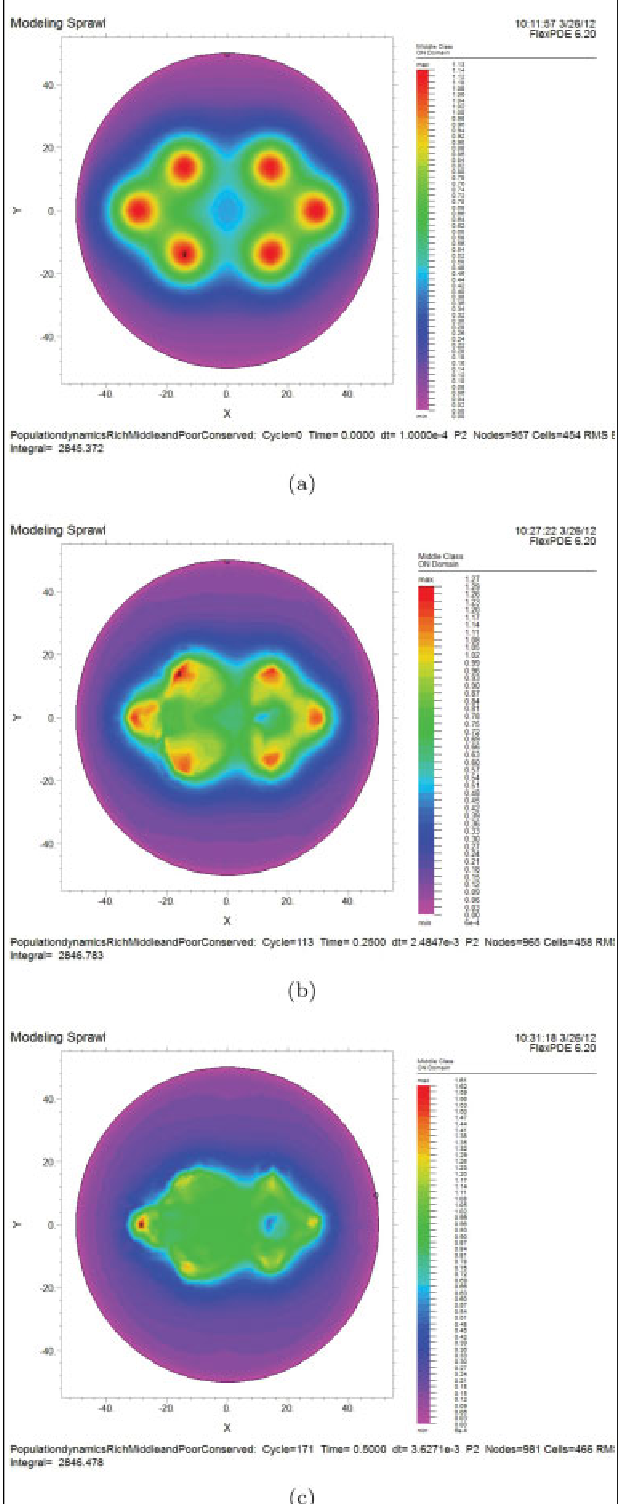
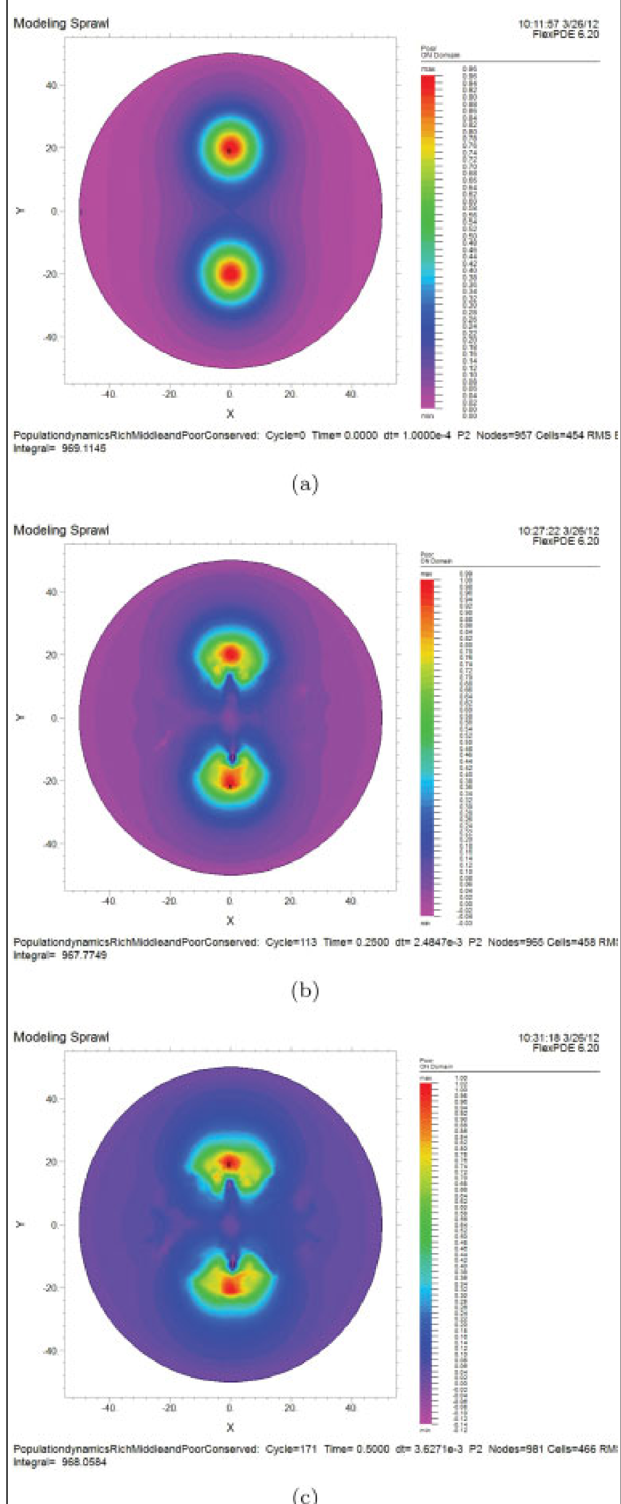
FIGURE 3



Contour plots of middle class density at the initial, intermediate, and final time instants for scenario 1.

FIGURE 4



Contour plots of poor density at the initial, intermediate, and final time instants for scenario 1.

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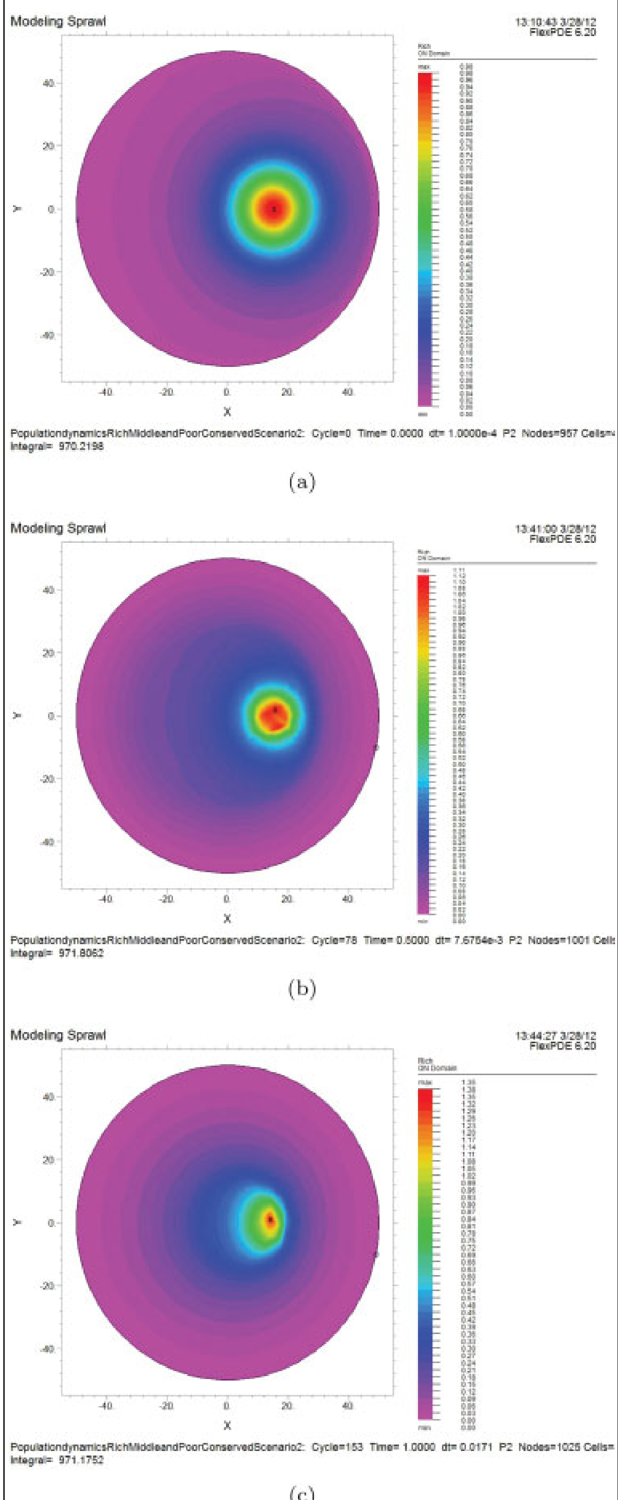
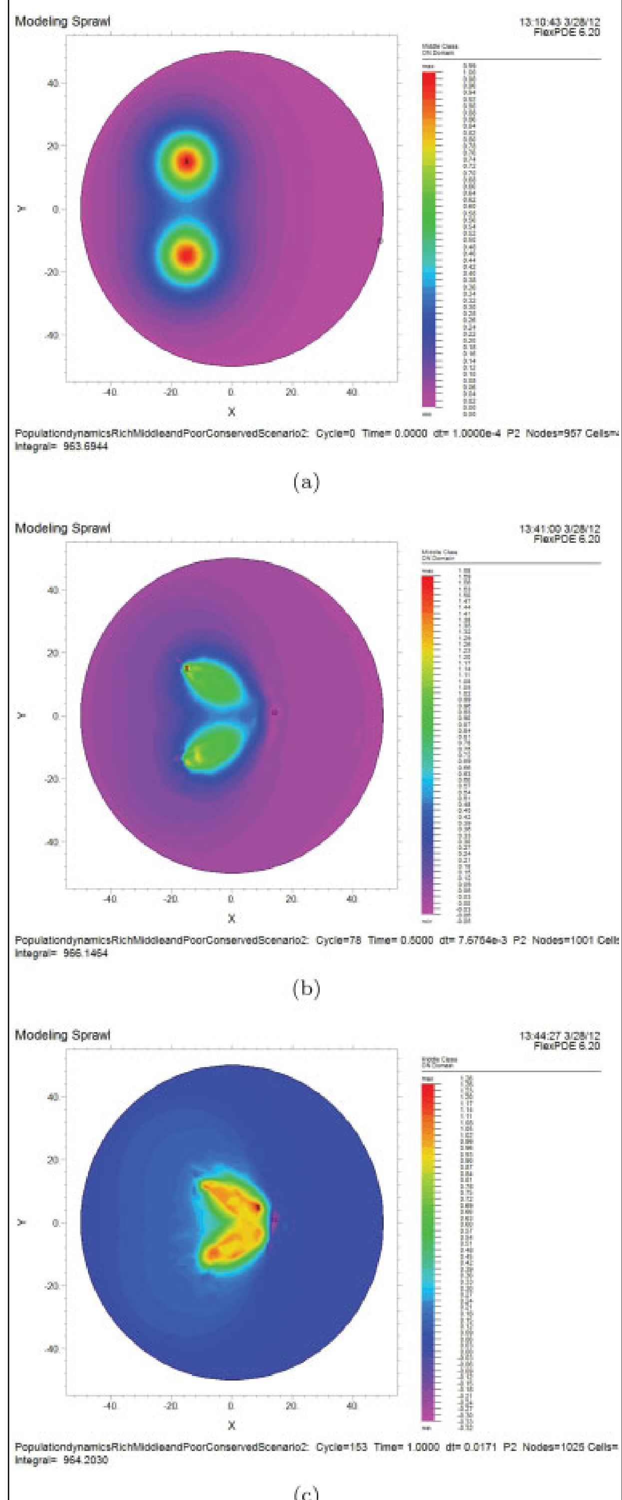
FIGURE 5



Contour plots of rich density at the initial, intermediate, and final time instants for scenario 2.

FIGURE 6



Contour plots of middle class density at the initial, intermediate, and final time instants for scenario 2.

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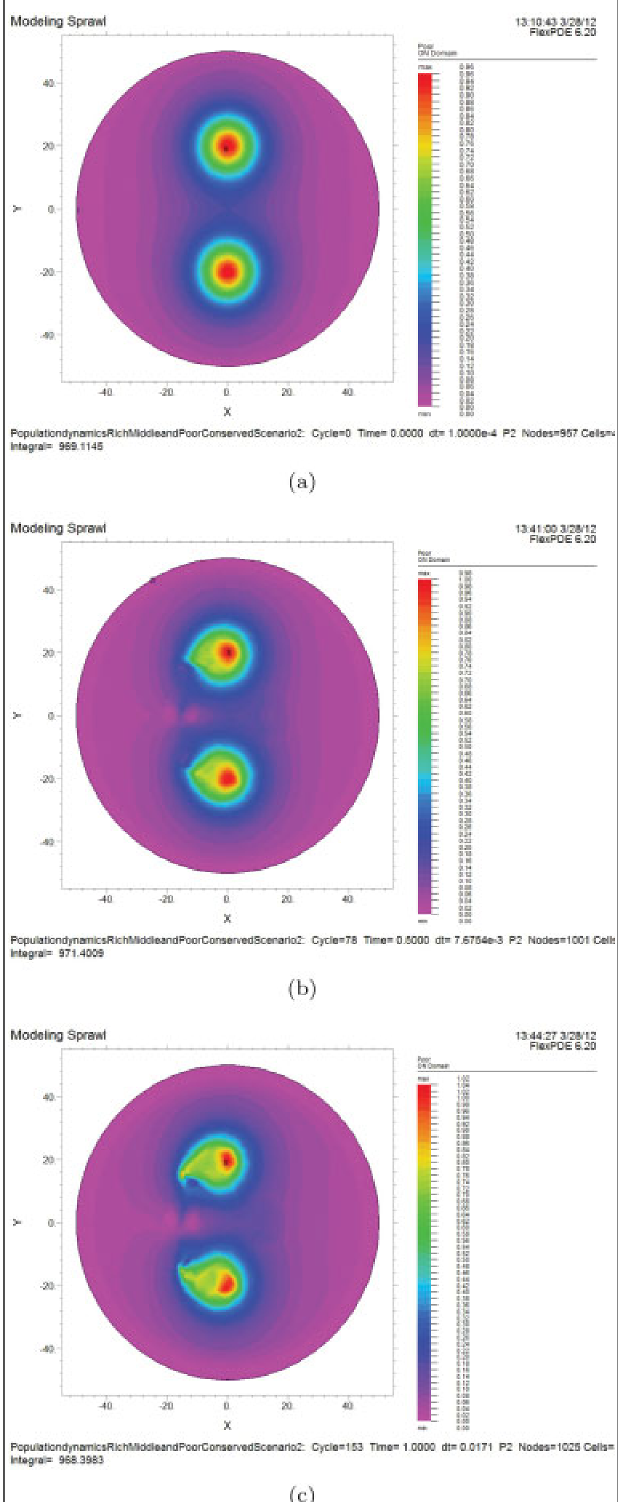
FIGURE 7



Contour plots of poor density at the initial, intermediate, and final time instants for scenario 2.

to a linear approach. Modeling the evolution of actual population leads to an agent-based model which is highly nonlinear. The actual population in a two-dimensional region D is the volume subtended by the density function on the region D in the $x-y$ plane, that is, $P(t) = \iint_D \rho(x,y,t)dxdy$.

2. We were only interested in modeling the evolution of the population densities of rich, middle class, and poor populations, as governed by mobility rules that were built into a nonlinear vector field f. Even though the vector field f is nonlinear, the evolution of a population density according to f is linear. In addition, we are not interested in modeling population growth or decay, and hence the total population (which is the volume subtended by the density on the entire domain) is a constant independent of time, that is, $P_{\text{total}}(t) = \iint_\Omega \rho(x,y,t)dxdy \equiv C(\text{ constant })$. Such a conservation property is automatically built into the continuity equation.
3. We assumed that there was no influx or outflux of the population through the boundary of the domain under consideration. This means that the population density at all inflow on the boundary of the domain was zero. Mathematically, this meant that we needed to impose a homogeneous Dirichlet boundary condition at the inflow points on the boundary of Ω (see Eq. (6)).
4. We assumed that the domain $\Omega \subset \mathbb{R}^2$ had a smooth boundary such that every point on the boundary had a well-defined outward unit normal vector.

8. MODEL AND SIMULATION RESULTS

We programmed the order parameters for the vector field $f(x)$ for rich, middle, and poor populations as follows:

1. *Rich*: The rich seek to move toward the rich if the value of rich density $\rho_R(x,y,t)$ is lesser than a predetermined rich high threshold t_R^H. We pointed the vector field for rich $f_R(x,y)$ toward the gradient of initial rich density $\rho_0^R(x,y)$, that is, $f_R(x,y) = \nabla \cdot \rho_0^R(x,y)$. We also multiplied the vector field $f_R(x,y)$ with a positive scalar quantity that we call rich mobility m_R. Otherwise, the rich stay put, that is, $f_R(x,y) = (0,0)^T$.
2. *Middle Class*: In regions where the middle class density $\rho(x,y,t)$ is between a predetermined low and high threshold (t_M^L and t_M^H), if the absolute difference between middle class and rich in those regions is within a predetermined rich low threshold t_R^L, then the middle class will move toward the rich, and hence, we point the middle class vector field in those regions toward the gradient of the initial rich density $\rho_0^R(x,y)$ (i.e., $f_M(x,y) = (\nabla \cdot \rho_0^R(x,y))$. If the absolute difference is not within t_R^L, then the middle class moves in the direction of gradient of initial middle class density $\rho_0^M(x,y)$, that is, $f_M(x,y) = \nabla \cdot \rho_0^M(x,y)$. In all other regions including the region where the rich density is larger than t_R^H, the middle class will not move, and

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hence $f_M(x, y) = (0, 0)^T$. We also multiplied the vector field $f_M(x, y)$ with a positive scalar quantity that we call middle class mobility m_M.

3. *Poor*: If the poor density $\rho_P(x, y, t)$ is larger than a certain poor high threshold ρ_P^H, then the poor vector field $f_P(x, y)$ is zero in that region. Otherwise $f_P(x, y) = \triangledown \cdot \rho_0^M(x, y)$, that is, the poor move in the direction of the gradient of the initial middle class density. In a similar manner as above, we used a scalar multiple m_P to model the mobility of the poor.
4. *Mobility*: We chose a scalar quantity to model the mobility because that would increase or decrease the actual velocity of movement at each point $(x, y) \in \Omega$.
5. *Domain*: We chose the domain Ω to be a circular region of radius 50 units.
6. *Initial distribution*: We chose an initial distribution of rich, middle class, and poor densities. We used the Cauchy distribution (could have used any distribution) to create bump functions centered appropriately.

The first scenario of initial distribution is chosen as follows: $\rho_0^R(x, y)$, the initial rich density was chosen to be a single bump at $(15, 0)$. $\rho_0^M(x, y)$, the initial middle class density $\rho_0^M(x, y)$ was chosen to consist of six bumps on an ellipse centered at $(0, 0)$. The initial poor density was chosen to be two bumps (one at $(0, 20)$ and another at $(0, -20)$). The spread of the bumps were chosen so that there was not much of overlap. FlexPDE simulation software was used to simulate the continuity equation programmed with the above mobility rules. (To view or download the model, visit `http://www.personal.kent.edu/~mdball/macro_model.htm`.)

The first set of plots Figures 2–4 (shown above) is the contour plot of the density of rich, middle class, and poor at three time instants (initial, intermediate, and final) where the initial time instant shows the initial distributions according to the first scenario. The second set of plots Figures 5–7 is the contour plot for density of rich, middle class, and poor for three time instants, where the initial time instant is according to a second scenario.

It is clear that with the mobility rules that we set above, the rich are moving closer to the rich. The middle class, because of the specific initial distribution of six bumps that we chose for scenario 1 Figures 2–4, are becoming more or less homogenous, except for a small blue region where the rich dominate. In scenario 2 Figures 5–7, the middle class are moving closer to the rich or toward each other. Most of the poor stay put except for some that tend to move toward the middle class. The same clustering and spatial segregation of affluence was noticed in the Summit Sim model. Hence the agent-based rules that were tested in Summit Sim have been translated into macroscopic movements, and the results are very similar.

9. CONCLUSIONS

As we hope our demonstration has sufficiently suggested, the continuity equation has the ability to extend synergetics in the macroscopic modeling of complex, self-organizing social systems; particularly in the case of social systems where the transport of agents/cases can be modeled spatially, such as residential mobility. The continuity equation accomplishes this task by conceptualizing order parameters as the macroscopic mobility of population densities. More concretely, our simulations showed that the microscopic rules that led to spatial segregation in our agent-based model, Summit Sim, could be translated into movements toward the gradient of the initial distribution of densities, depending on certain threshold conditions. As we have stated several times now, we believe that such an approach assists agent-based and case-based modeling by (1) linking macroscopic and microscopic modeling; (2) transforming the dynamics of highly nonlinear vector fields into the linear motion of densities; (3) letting predictions to be made about future states of a complex system; and (4) allowing formalization and generalizations to be made to similar complex systems.

We do, however, need to mention the following drawbacks for using the continuity equation as a model of mobility: First, like always, it is not possible to model complex systems that exhibit chaotic behavior due to the inherent sensitivity of the qualitative behavior of solutions to initial conditions and parameters. Second, the continuity equation can be used only when some idea of the average behavior (over time) of the agents in an agent-based model is known. The vector field f is static (i.e., time independent), and hence the predictions of the model are valid only under the assumption that the average same mobility rules are obeyed. This can also be thought of as an advantage of the method, since educated guesses for the average mobility rule can be simulated and the solution of the agent-based model and the continuity equation can be compared. Finally, finite element-based simulators such as FlexPDE are commercially available for simulations on two- and three-dimensional domains (more so for 2D). The continuity equation being a PDE has the same numerical limitations as simulating any other PDE. Fortunately, there exist a lot of situations which can be modeled macroscopically as the motion of densities in 2D.

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