1.16 Agent-Based Modeling

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Glossary

Agent-based modeling A computer simulation comprising of multiple types of heterogeneous agents which are autonomous decision-making entities (e.g., cars). Agents are given specific rules for interaction with other agents and/or other entities within a system. Through such rules and interactions, more aggregate patterns emerge (e.g., traffic jams).

Big data Big data not only refers to datasets that are unusually large in volume, but those that also exhibit other properties that distinguish them from "traditional" datasets. These include *velocity* (data that are generated rapidly and might only be relevant for a short amount of time), *variety* (data that are stored in various formats and hold diverse pieces of information), and *veracity* (there are uncertainties around bias, noise, and the level of representation) (Croitoru et al., 2014). Examples include established datasets such as national censuses to mobile phone data or social media data.

Bottom-up modeling The notion that changes at the global or macro-level are driven from interactions that occur at the lowest micro-level. For example, in Schelling's (1971) classic segregation example, an individual's preference for who they live nearby drives the patterns of segregation that occur at a neighborhood level.

Bounded rationality In decision making, individuals or agents do not have universal knowledge. Their decisions are limited by the information that they have which is often specific to their context, the time they have to make their decisions, and their cognitive abilities (Simon, 1955).

Calibration This is the process of adjusting model parameters so that the behavior of the model closely matches some observed (often historical) conditions (O'Sullivan, 2004). This is also known as "fitting" the model to some observed data (Gilbert and Terna, 2000).

Complexity Complexity arises when a small number of rules or laws, applied at a local level and among many entities, are capable of generating complex global phenomena: collective behaviors, extensive spatial patterns, hierarchies, etc. are manifested in such a way that the actions of the parts do not simply sum to the activity of the whole.

Emergence The product of interactions between individuals, for example, an exchange of information. From these interactions new patterns, processes, or information is produced. What is central to the idea of emergence is that what emerges cannot be predicted. As Aristotle noted, "*the sum is greater than the parts*".

Validation Validation is the next process after calibration and its main purpose is to demonstrate that the model is sufficiently accurate given the context of the system that it is attempting to simulate. This is often achieved through applying the model to unseen data to test that it can produce the correct output.

1.16.1 Introduction

Understanding individual behavior patterns, their causes, and their consequences has been an issue that has taxed geographers for the last 50 years. Early approaches such as Alonso's (1964) bid rent model and Hagerstrand's (1967) diffusion model had one central common intellectual caveat: in order to say something useful about social systems, analysis had to take place at the aggregate level (Heppenstall et al., 2012). Viewing the world in this manner meant that geographical systems were distilled down into homogeneous units whereby it was virtually impossible to say anything meaningful about their inner workings or microdynamics (Batty, 2008).

New forms of "big" data and simulation methods are beginning to give greater insight into the complexity inherent within geographical systems and to reveal the role of the individual. This understanding is being reflected in the way that geographical systems are currently being conceptualized. Instead of large, aggregate models that contain equations applied to homogeneous groups, recent thinking emphasizes the individual, in particular their networks and interactions, as being one of the most important factors that shape geographical systems (Batty, 2013). For O'Sullivan et al. (2012) these interactions and decisions can potentially be seen as the drivers of social systems. If we can piece together knowledge about *who* is making these decisions and *what* influences them, we can advance on the previous 50 years of geographical modeling by being able to both pose and answer important questions about the causes and consequences of individual behavior patterns.

Leveraging this information about individuals and their interactions will hopefully give researchers a clearer understanding about the role that complexity plays in shaping geographical systems. The definition of a complex system encompassing "heterogeneous subsystems or autonomous entities, which often feature nonlinear relationships and multiple interactions" (An, 2012) is closely aligned to the description that we would assign to geographical systems. Complexity theory is still in its early days with advancements required in the "onotological and epistemological representations" of complexity (An, 2012; Grimm et al., 2005; Manson and O'Sullivan, 2006; Parker et al., 2003). The merger of concepts from complexity, agent-based modeling (ABM), and big data has the potential to create a new deeper understanding of the mechanisms powering geographical systems.

To do this we need to use tools that can exploit these new forms of data to create detailed simulations of the main components and drivers of geographical systems. Perhaps most importantly, these methods need to be able to simulate behaviors and interactions at the individual level. An individual-based method that has seen a rapid uptake by researchers across the social and geographical sciences in the past 20 years is ABM (Macal, 2016). ABM advocates the creation of individuals with their own attributes and behaviors. The emphasis within these models on the individual makes it a natural framework to apply within social and geographical systems. Its popularity has been cemented by increases in computer processing power and data storage along with developments in computer-programming languages and easily accessible frameworks that enable rapid development of models with minimal programming experience.

ABM has now reached a point of acceptance as a research tool across the geographical and social sciences with numerous journal articles and books dedicated to applications and developments (see, e.g., Batty, 2005; Benenson and Torrens, 2004; Gimblett, 2002; Heppenstall et al., 2012; Railsback and Grimm, 2011). Furthermore, the recent emergence of big data is beginning to have a large impact on ABM (Heppenstall et al., 2016). The proliferation of novel, high-resolution, individual-level data sources provides ABM with an opportunity to address some of the more critical methodological issues, namely construction of accurate individual-level behavioral rule sets and robust model calibration and validation. Whether this opportunity is taken up is yet to be seen. What is clear is that researchers now have the data and tools at their disposal to examine geographical systems in unprecedented individual-level detail, thus creating new knowledge and understanding about how these systems evolved and what the consequences of future individual behaviors are likely to be.

This article presents an overview of how ABM is being utilized for the simulation of geographical systems. We have attempted to be as comprehensive as possible given the space available, but will have inevitably omitted important aspects. In this article, we have attempted to find a balance by including what we consider to be the key elements of ABM with respect to geographical systems and providing extensive references for interested readers to follow up on any of our discussion. We begin in section "**The Rise of the (Automated) Machines**" by providing a brief overview of the development of agent-based models, before moving on to defining agents in section "**What Is ABM?**" and how they can be developed to incorporate human behavior. Section "**Steps to Building an Agent-Based Model**" walks through the process of how to design and build agent-based models including steps for verification, calibration, and validation of such models. For geographers, the influence of space on agents is one of the key factors that we need to account for; rationale and guidance on integrating agent-based models with geographical information systems (GIS) is given in section "**Integrating GIS and Space Into Agent-Based Models**" along with a range of applications where agent-based models have been applied. Finally, we discuss what the main challenges for ABM are in section "**Challenges and Opportunities**" before offering concluding thoughts in section "**Conclusion**".

1.16.2 The Rise of the (Automated) Machines

ABM owes much of its unique character to ideas and concepts borrowed from other disciplines. For example, one of the key strengths of ABM is the ability of individual agents to be autonomous, that is, have full control over their future decisions. This part of an ABM's DNA owes much to early work on digital computers, such as Lovelace (1843) and Turing's (1936) work on the computability of mathematics and von Neumann's (1951) early work on computer design. As Torrens (2000) points out, the intelligence that is endowed on agents, such as the ability to reason, can also be seen as drawing on ideas from cybernetics (Weiner, 1948) and intelligent machines (Turing, 1950).

Agent-like models first began to make an appearance in the academic literature in the 1960s and 1970s. Prior to this, the most common approaches to simulating and gaining new insight into geographical systems were through the use of more established mathematical and statistical models such as system dynamics, spatial interaction (e.g., Fotheringham and O'Kelly, 1989), or diffusion models (Hagerstrand, 1967). In spatial interaction models, for example, large diverse groups of people were treated as one homogeneous (aggregate) group and all given the same behavior and movements (Wilson, 1974). The main criticisms leveled at these approaches were that the rich variability inherent within many data forms was lost through the process of aggregation. While these approaches can and have been used to successfully predict macro-level patterns of behavior (e.g., Batty, 1976; Birkin et al., 1996), they struggle to give any insight into why these behaviors appeared and how they might manifest themselves in the future. Perhaps most importantly for geographers wishing to understand the impact of individual behavior, these methods are incapable of simulating individuals, their interactions, and the resulting consequences.

The first automata models that focused on modeling geographical phenomena came from the area of cellular automata (CA). The basic features of a CA have been well documented within the literature (see Wolfram, 2002 for a thorough overview). Essentially, a CA is a discrete dynamic system with the behavior specified in terms of local relationships with space represented as a grid (i.e., a lattice) containing cells of equal size. The cell state (e.g., a value of either 0 or 1) is determined by the state of its neighbors, by a set of local rules, and by the cell itself (see Benenson and Torrens, 2004; Iltanen, 2012; Wolfram, 2002) as illustrated in **Fig. 1**. From a geographical perspective, the first notable use of a CA was for the purpose of urban growth and land use (e.g., Nakajima, 1977; Tobler, 1979). Due to the relative ease of implementation, CA modeling remains a popular choice for simulating large-scale urban phenomena such as urban sprawl (Al-Ahmadi et al., 2009; Clarke et al., 1997; White and Engelen, 1993).

Related to CA is microsimulation. With its origins in economics (Orcutt, 1957), this approach has been widely used to study the impact of social, administrative, or environmental changes on populations. This methodology is commonly used to create small area microdata such as individual-level synthetic populations. **Fig. 2** shows how individual-level data, such as the Sample of Anonymised Records (a sample of individual-level data from the UK Census) for a given spatial area, are used to create

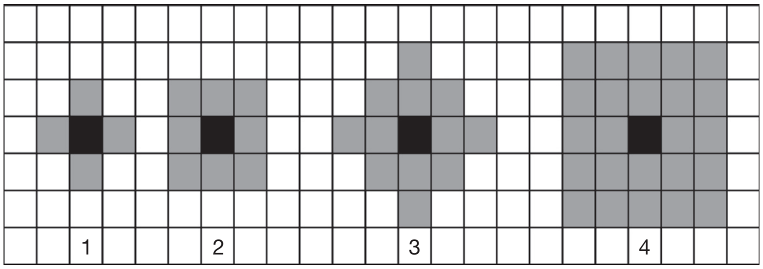

Fig. 1 Diagrammatic representation of 2D CA and the most commonly used neighborhoods (1) von Neumann 1-neighborhood, (2) Moore 1-neighborhood, and extended (3) von Neumann and (4) Moore neighborhoods.

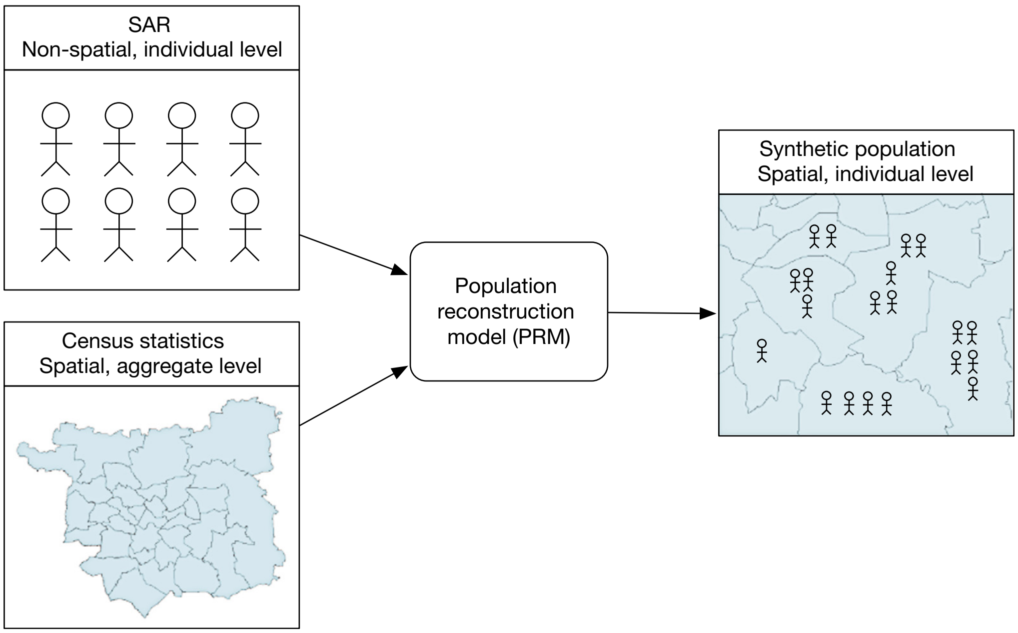

Fig. 2 Schematic outlining of the basic process of creating a synthetic population using microsimulation.

a representative synthetic population of that area. Transition probabilities, such as the likelihood of an individual giving birth, are then applied to each individual unit to generate future scenarios (see Harland et al., 2012 for a discussion of the different methods used to achieve this). As with CA, microsimulation operates at the level of the individual to simulate the global consequences of local interactions while allowing the characteristics of each individual to be tracked over time. Microsimulation has been widely taken up in geography with applications within transport (e.g., MATSim (Horni et al., 2016) and TRANSIMS (Nagel et al., 1997)), population dynamics (e.g., SimBritain, Ballas et al., 2005), and health (e.g., Smith et al., 2011). Wu and Birkin (2012) provide a detailed overview of the diversity of spatial applications of microsimulation (along with noting how such an approach could be leveraged within agent-based models).

While both CA and microsimulation allow the simulation of individuals, they do contain several drawbacks. CA models tend to be spatially constrained to a grid and, although each cell can be in a different state, they are all driven by identical transition rules. This makes it impossible to capture a range of unique individual behavioral traits. Microsimulation only allows the modeling of one-direction interactions: the impact of the policy on the individuals. With microsimulation there is no behavioral modeling capability (as everything happens through transition matrices) and perhaps most importantly, individuals do not interact with each other (Gilbert and Troitzsch, 2005). The ability to create individuals with multiple attributes and behaviors who can move freely within a space and interact with other individuals is critical if we are to create tools that allow new insight into the dynamics and processes of geographical systems and to understand the impact of individual patterns of behavior.

ABM is a methodology that inherently possesses these key elements. It arrived at a time where computing power and storage were rapidly increasing along with new developments in object-orientated computer-programming languages that were well suited to the development of agent-based models. It is at this point in the 1990s that ABM trickled into the social sciences, most notably through the work of Epstein and Axtell (1996) who demonstrated how agent-based models could be extended from modeling people to growing entire artificial societies—an area that they termed *Generative Social Science*. Because ABM generates emergent phenomena from the bottom-up, it raises the issue of what constitutes an explanation of such a phenomenon. According to Epstein and Axtell (1996):

> [ABM] may change the way we think about explanation in the social sciences. What constitutes an explanation of an observed social phenomenon? Perhaps one day people will interpret the question 'Can you explain it' as asking 'Can you grow it?'

It is this thinking that has percolated into the ABM community leading to new ways of examining geographical systems, "not from a traditional modeling perspective but from the perspective of redefining the scientific process entirely" (Bonabeau, 2002). Rather than favoring deduction (testing of assumptions and their consequences) or induction (the development of theories on the basis of observations), there is a *third way* (Axelrod, 1997). The researcher starts with a set of assumptions, but then employs experimental methods to generate data that can be analyzed inductively (Gilbert and Troitzsch, 2005).

1.16.3 What Is ABM?

As discussed in section "**Introduction**", the development and acceptance of ABM is the result of several different strands that include the development of automata approaches (e.g., CA) and object-orientated programming languages such as C++. These key elements coevolved with developments in increased processing power, data storage, and the proliferation of large amounts of individual-based data that have shaped ABM even further. In this section, we examine the components identified within the common definitions of ABM to see if they hold with current ABM design and practice. A particular focus is how these definitions fit with ABM that are routinely applied to geographical systems; do our commonly held definitions need to shift to ensure that we able to "facilitate the exploration of system processes at the level of their constituent elements" (Crooks and Heppenstall, 2012)?

Despite the rapid proliferation of ABM, there is surprisingly no universal definition of an agent-based model. While definitions often have several commonalities, normally related to their function (see **Table 1** for a description of these), the sheer diversity of applications makes anything more than a loose definition of ABM seemingly impossible (see Macal, 2016). Far from this being problematic, this is reflective of the broad framework which has promoted the vastly different applications that can be designed and built (as will be highlighted in section "**Integrating GIS and Space Into Agent-Based Models**"). One of the most "popular" and early definitions of ABM heralds from a computer science perspective. Wooldridge (1997) defined agents as "*an encapsulated computer system that is situated in some environment and that is capable of flexible, autonomous action in that environment in order to meet its design objectives*". While easily accessible, Wooldridge's definition is broad in scope, prompting Jennings (2000) to give further clarification emphasizing that agents should have a specific goal and be embedded within an environment within which the agents receive inputs. In addition, they should have control (*autonomy*) over their internal state and behavior that allows them to be *reactive and flexible* in pursuit of fulfilling their objectives. These two definitions together clearly articulate a view of ABM from a technical perspective with the emphasis on the DNA of the agents.

Other definitions have emphasized the value of agent-based models in providing new knowledge and understanding about the dynamics of the real-world through their ability to evolve and interact, allowing unanticipated actions and behaviors to emerge from a computer simulation (Crooks and Heppenstall, 2012). Here, concepts such as emergence and bottom-up modeling

Table 1 Core components of an agent: drawn from Wooldridge and Jennings (1995), Epstein (1999), Bonabeau (2002), Macal and North (2005), Crooks et al. (2008), Crooks and Heppenstall (2012), and Torrens (2012)

Component	*Description*
Autonomy	There is no central control over agents—they are essentially masters of their own fate
Heterogeneity	Each agent can potentially have their own unique attributes and rules
Explicit space	Agents "exist" within some form of space: this can be a physical environment or more abstract (e.g., social network)
Interactions	Agents can interact with other agents exchanging information
Bounded rationality	Agents do not have universal knowledge, only that specific to their context
Reactivity	Each agent should be able to proactively respond to changes in their environment

dominate the descriptions of the agents. For Bonabeau (2002), it is the ability of ABM to handle emergent phenomena that sets ABM apart from other approaches and allows agents to provide a natural description of the system.

While including the more technical attributes of agents, these definitions also emphasize the heterogeneity of agents, with individual variations being accounted for by random influences (Helbing and Balietti, 2011). A slightly different perspective is taken by researchers whose ABMs are embedded within spatial systems. Here the emphasis is placed on the ability of agents to move and interact with each other and the environment at the micro-level (neighborhood), producing emergent behavior that can only be revealed by viewing the system from a higher geographical (macro) scale (Crooks et al., 2008; Malleson et al., 2010). For spatially explicit applications, the influence of space is equally important to agent movement and interactions (e.g., Parker et al., 2003; Pires and Crooks, 2017).

Fig. 3 diagrammatically represents some of these core "components." Here, two heterogeneous agents are situated in their own distinct spaces within an artificial world. These spaces could be specific geographical areas which exert their own environmental influences on the agents, for example, the availability of a particular service. Through the direct interaction, the agents exchange information which can lead to the emergence of new knowledge or ideas. This newly "emerged" knowledge may result in the agent reacting and pursuing a new form of behavior/decision making to reach its goal.

To give a simple example of how these characteristics come together within an ABM and how micro-level agent *choices* lead to macro-level patterns emerging, consider the simple segregation model of Schelling (1971); one of the earliest ABMs. Within this model there are two types of agents (*green* and *yellow*) as shown in **Fig. 4**. Each agent is autonomous and possess a desire to live in a neighborhood (defined by its eight surrounding cells), with a percentage of neighbors who are identical to themselves. In this example, the agent preference for similar neighbors was set at 30% (i.e., at least 30% of an agent's neighbors must be of the same type for the agent to be satisfied). Initially the agents are randomly distributed throughout the environment. Agents move (i.e., take an action) if they are in a situation where their neighborhood preferences are not met (i.e., the condition to move). Over time, agents move to empty areas (the black cells) and segregated neighborhoods emerge at the aggregate level.

While it is unsurprising that the level of segregation increases with individual preferences for similar neighbors, it *is* surprising that communities still self-segregate even when the preference for similar neighbors is relatively low (e.g., 30%). This is illustrated in **Fig. 5**. The utility of such a model is that it demonstrates that aggregate patterns cannot always be easily discerned from the

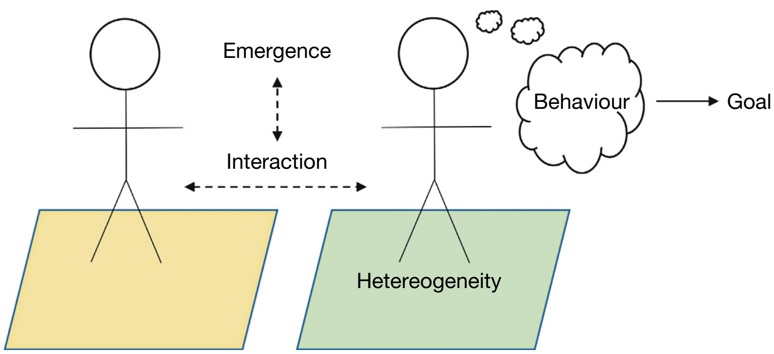

Fig. 3 Schematic illustrating of some of the main components of an agent.

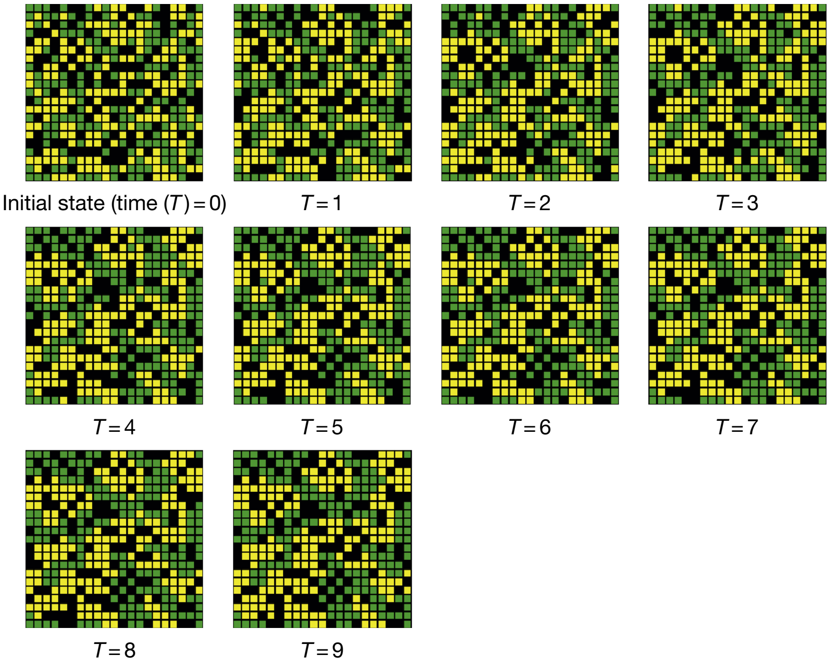

Fig. 4 Progression of segregation—agents want to live in a neighborhood where 30% of their neighbors are the same color.

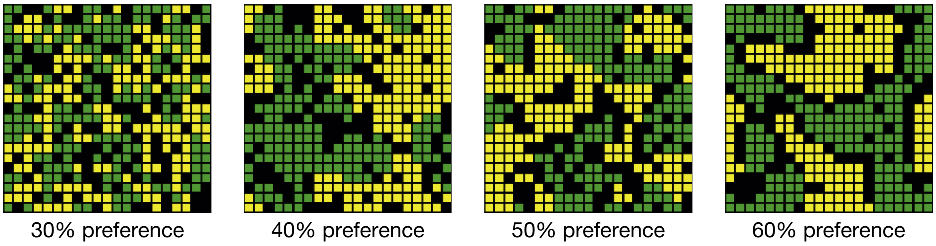

Fig. 5 Examples of how changing agents' neighborhood preference leads to different patterns of segregation emerging.

behaviors of the individual agents—the sum is greater than the parts. While this is a simple example, such mild tastes and preferences for certain neighborhood types have been shown to cause "real" world segregation to emerge (see Benenson et al., 2002). This example also serves to show the importance of being able to capture and represent emergent phenomena in geographical systems. Without the ability to model this property through individuals and bottom-up modeling, we cannot fully understand the dynamics and processes within our systems of interest.

Finally, while there is a broad consensus in the core characteristics that an agent should contain, the application area and the research agenda of the developer exert the greatest influence over the overall form of the agent, and thus its definition. For example, Heppenstall et al. (2005) linked an agent-based model to established geographical (spatial interaction) and artificial intelligence (AI) inspired (genetic algorithm) models to handle influences of space, and to optimize agent behavior. The agents within this application could equally be described as being hybrid, spatially explicit, or optimizing, highlighting how easily other definitions can be assigned to agent-based models. With the increase in big data and the new insights into individual behavior that they offer, researchers will be able to pose increasingly complex questions about how social systems work and how they will evolve in the future (as will be discussed in section "**Challenges and Opportunities**"). It is likely that the agent-based models that they build to answer these questions will absorb the characteristics of these new forms of data, thereby generating new essential components within an agent design and definition.

1.16.3.1 Making Agents More Human

While we provided an overview of the core components of an agent and how the ABM paradigm perfectly aligns with simulating individuals in geographical systems, how do we capture and embed the behavior that makes us unique into these models? Humans are in possession of such diverse personality traits, varying levels of knowledge, experience, desires, and emotions (common set of emotions: interest, joy, happiness, sadness, anger, disgust, and fear (Izard, 2007; Bonabeau, 2002)) that attempting to simulate any small aspect of this seems a foolish endeavor. Fortunately for the modeler, it is rare that we wish to simulate the full spectrum of human behavior. Instead, we are often interested in one or two clearly defined aspects of behavior that we believe has a strong influence on the system under investigation. Therefore in order to simulate human behavior, researchers embed behavioral frameworks into their ABMs (see Kennedy (2012) and Balke and Gilbert (2014) for an overview). These frameworks can be broadly categorized into two areas; mathematical and cognitive. Examples from each category are presented later to demonstrate their utility.

Mathematical approaches range from the use of random number generators to select between predefined choices (e.g., Gode and Sunder, 1993), or the use of threshold-based rules and complex probabilistic rules sets. Due to its ease of implementation, one of the most commonly used approaches is that of threshold-based rules. Threshold rules come into operation when a preset value is exceeded. Depending on the value, this will result in behavior from a predefined set. For example:

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IF <hunger> is below <hungerThreshold1> THEN agent-dies
IF <hunger> is above <hungerThreshold2> THEN address another goal
IF <hunger> is between <hungerThreshold1> and <hungerThreshold2> THEN search-for-food
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Adapted from Kennedy (2012).

Examples of the use of this approach for geographically explicit models can be found in Heppenstall et al. (2005) and Crooks (2010). While such rule sets are able to broadly simulate behavior, one of the main criticisms leveled at this approach is that it cannot easily account for the multiple components of human behavior and they should only be used when behavior can be well specified. An alternative approach that can readily handle more complex behavior comes from the category of cognitive frameworks.

Perhaps the most popular architecture used is the Beliefs–Desires–Intentions (BDI) modeling framework (Bratman et al., 1988; Rao and Georgeff, 1991). This architecture has been used in several areas, including air traffic management systems (Rao and Georgeff, 1995), simulations of geopolitical conflicts (Taylor et al., 2004), land-use planning (Caillou et al., 2015), and frameworks for models of crime reduction (Brantingham et al., 2005a,b). Despite its uptake, the BDI framework has been widely criticized as being too restrictive while others feel that they are overly complicated (Rao and Georgeff, 1995). Fundamentally, the framework assumes rational decision making, which is difficult to justify because people rarely meet the requirements of rational choice models (Axelrod, 1997). Brailsford and Schmidt (2003) see the restriction of the framework to cognitive processes as a limitation; the BDI framework cannot integrate physical, emotional, or social processes or the interactions between them. Balzer (2000) also notes that the core elements are difficult to observe directly: observation can only be achieved in a laboratory setting which is unlikely to relate to real situations.

A cognitive framework that can overcome these limitations is the PECS framework (physical conditions, emotional states, cognitive capabilities and social status). Proposed by Schmidt (2000) and Urban (2000), this architecture states that human behavior can be modeled by taking into account physical conditions, emotional states, cognitive capabilities, and social status. The framework is modular, in the sense that it allows the modeler to separate components that control each aspect of the agents' behavior (Martõnez-Miranda and Aldea, 2005). To illustrate the PECS framework features, an example proposed by Urban (2000) is adapted here. Consider a person in a shop who is contemplating purchasing some goods. They might experience physical needs (such as hunger), emotional states (such as surprise at the available goods), cognition (such as information about current prices), and social status (which will, e.g., affect how the agent reacts to the shop assistant). Schmidt (2000) and Urban (2000) argue that every aspect of human behavior can be modeled using these components although, depending on the application, it might not be necessary to incorporate all of them (Schmidt, 2002). Recent examples of successful integration of this approach into geographically explicit agent-based models include that of Malleson et al. (2010) and Pires and Crooks (2017).

While these frameworks are representative of the two broad approaches that modelers use for simulating behavior in agents, the number of alternative architectures that are appearing is rapidly increasing (e.g., Gigerenzer and Goldstein, 1996). However, regardless of the complexity of these frameworks, they are equally reliant on access to detailed individual-level data and rigorous calibration and validation for their results to be valid. How we calibrate and validate these models, as well as an overview of the data that we can use is presented in the following sections.

1.16.4 Steps to Building an Agent-Based Model

> … although ABM is technically simple, it is also conceptually deep. This unusual combination often leads to improper use … .
>
> Bonabeau (2002).

ABM is an extremely powerful methodology. As shown in the sections earlier, and will be demonstrated in the following sections, it is technically possible to incorporate a vast array of complicated individual behavioral frameworks, voluminous interactions, complex psychology, intricate (spatial) environments, and many other advanced modeling features that are typically extremely difficult to account for when using aggregate modeling methods. However, this flexibility is tempered by the risks of creating over-complicated models. Models that have been poorly designed or inadequately validated have the potential to be no easier to understand than the underlying system that they are attempting to simulate (Crooks et al., 2008).

To mitigate these risks, the ABM community has developed a suite of approaches that can inform the design, implementation, and testing of models to make them more robust. These include innovative means of validating models (e.g., pattern-oriented modeling, Grimm et al., 2005), standard approaches to the design and documentation of models, for example, the Overview, Design concepts, and Details (ODD) protocol (Grimm et al., 2006, 2010) which has recently been extended to incorporate more options for describing human decision making (ODD+D; Müller et al., 2013), the application of computationally efficient methods to explore large parameter spaces (e.g., genetic algorithms, Malleson et al., 2009), and many others. This section will discuss some of these methods in order to illustrate best practice in building reliable agent-based models.

Fig. 6 presents an overview of the *typical* model design process. It is important to note that this is not the *only* process that a modeler might use in order to create their model. As with many features of ABM, there are a multitude of ways to approach the task of building a model. For more details, the interested reader should refer to any of the excellent ABM text books that are available such as Wilensky and Rand (2015) or Railsback and Grimm (2011) and for steps in modeling within the social sciences more generally see Gilbert and Troitzsch (2005). The remainder of this section will discuss each step in more detail: formulating a research question and designing an appropriate model (section "**Preparation and Design**"); implementing the model using a chosen tool (or suite of tools) as discussed in section "**Model Implementation**"; evaluating the robustness and accuracy of the model (section "**Evaluating a Model**"); and finally evaluating the robustness and accuracy of the model (section "**Evaluating a Model**") and the challenges that spatial models pose and how they can be overcome.

1.16.4.1 Preparation and Design

The first step in the modeling process is to define the research question (i.e., what element of the real-world are you interested in?). What, specifically, will be the aim and purpose of the model? At this stage, it is extremely important to decide whether ABM is a suitable approach. Although ABMs are potentially extremely powerful, they are also much more complicated to create than aggregate modeling methods, such as regression. This is partly due to the immaturity of the available tools (software packages such as SPSS

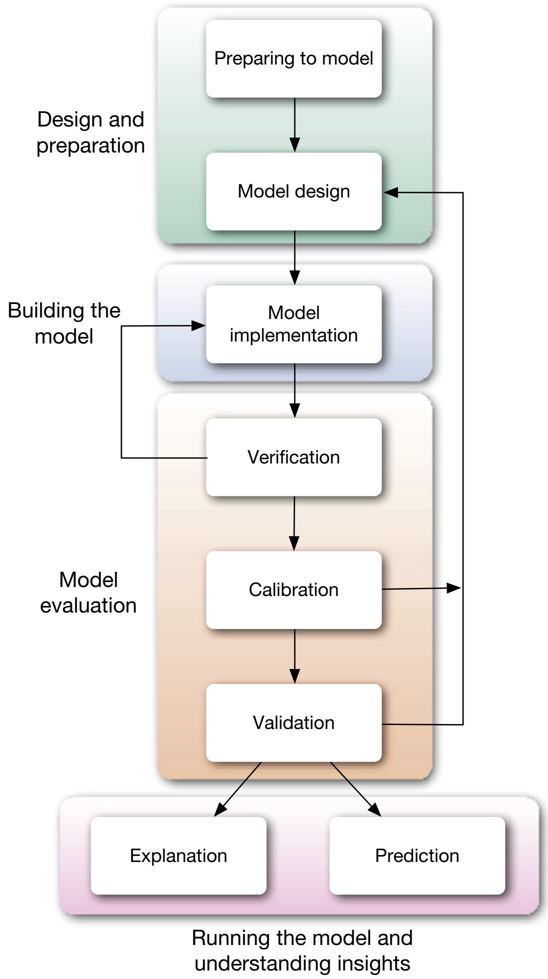

Fig. 6 An overview of the typical modeling process.

allow the user to run a multitude of mathematical models at the push of a button; equivalents do not exist for ABM) but also because the models themselves are considerably more complicated. It is therefore important to critically assess the target system under study, understand which factors are the most important drivers of the system, and therefore decide whether the advantages offered by ABM outweigh the additional difficulties. As an example, consider a model of air moving over the wing of an aircraft. The system consists of individual entities (air particles) and its aggregate properties (i.e., air motion, pressures, etc.) are dependent on the interactions between discrete particles. In this sense, it appears to be an ideal candidate for an ABM. However, in this case the behavior of the particles is effectively homogeneous and the system can therefore be modeled adequately with aggregate equations. There is no benefit to modeling the individual particles. That said, there are many systems in which the complex interactions that govern the real-world behavior make analytical solutions impractical or impossible (Bonabeau, 2002).

If the use of ABM is considered to be an appropriate approach, then the first design decision regards the level of abstraction of the model which depends on its purpose. Take the example of a map, the level of detail portrayed on the map is dependent on its purpose. For instance, a map intended for driving is generally less detailed than that of one for hiking as the purpose is different (Miller and Page, 2007). This is the same for modeling and there are typically two categories that the model will fall under: *predictive* or *explanatory*. With predictive modeling, the aim is to simulate a system with a degree of realism such that the results can be used empirically. A predictive agent-based model of a social phenomenon (such as crime, traffic, protests, etc.) might, for example, include a realistic representation of the underlying environment that allows the models to make predictions about the future state of the real-world directly. Explanatory modeling, on the other hand, is typically concerned with refining the theoretical explanations that explain a phenomenon. Explanatory models are often greater abstractions away from the real-world than their predictive counterparts. The Schelling (1971) segregation model outlined in section "**What Is ABM**?" is an excellent example of an explanatory model—it attempts to better understand a phenomenon but does not directly provide guidance about where or how the real system can be manipulated to reduce segregation.

Having broadly "prepared" for modeling by deciding on the approximate level of abstraction, the process in **Fig. 6** suggests that the next stage is to *design* the model. Wilensky and Rand (2015) describe this as "top-down" modeling; the designer comprehensively plans the characteristics and behaviors of the agents, designs the environment, and defines the possible interactions. However, an equally appropriate approach might be to begin implementing the model immediately, such that the design and implementation coevolve. In practice, most modelers will use some combination of approaches; for example, a broad design with specifics resolved during implementation.

Before discussing the implementation specifically, it is worth highlighting two important developments. The first is the ODD protocol (Grimm et al., 2006, 2010). The protocol formalizes the approach to documenting models with the aim of making it easier for others to understand and reproduce models. It is organized around the three main components that need to be documented: Overview, Design concepts, and Details. Modelers should to be aware of the protocol so that they can choose whether to make use of some or all of it when documenting their own models. The second development concerns the level of complexity of a model. It was highlighted earlier that a poorly designed agent-based model will be no easier to understand than the target system (i.e., the real-world) that it is attempting to model. Although most people agree that model complexity is not appropriate unless it is justified by the target system, opinions as to how to reach the "appropriate" level of complexity are polarized. The "Keep It Simple, Stupid" (KISS) argument (e.g., Axelrod, 1997) posits that models should be as simple as possible initially, with additional complexity added only if the model is unable to appropriately represent the system in its simplest form. The "Keep It Descriptive, Stupid" (KIDS) approach (e.g., Edmonds and Moss, 2004), on the other hand, is to *start* with a model that reflects the evidence and knowledge about the target system, however complex that it makes the model, iteratively remove features that appear to be unnecessary. Recent KIDS work has also explored the stages of this abstraction process in detail (Lafuerza et al., 2016).

1.16.4.2 Model Implementation

As noted earlier, implementing an agent-based model is usually considerably more involved than alternative, traditional modeling approaches. This is partly because there are no standard models that can be used "off the shelf"—every ABM is different and, given the complexity of the underlying systems that agent-based models attempt to simulate, a generic model would not work. However, in the last decade a number of toolkits have emerged that substantially reduce the difficulty required to implement models (this will be discussed in detail in section "**ABM Toolkits**"). That said, using an existing toolkit is not essential and there can be significant advantages to building a model from the ground up using conventional (object-oriented) programming techniques if a modeler has sufficient programming knowledge and experience. The advantage with using existing tools, rather than starting from scratch, is that the common elements that models require such as graphics libraries, common algorithms, data input/output procedures, and analysis tools need not be re-implemented.

Section "**ABM Toolkits**" reviews a number of toolkits that have been designed to support the implementation of agent-based models. Although most share similar features, some are easier to use (particularly for developers without any programming experience) and others are potentially more powerful (guidelines for assessing such frameworks are discussed in section "**ABM Toolkits**"). For example, Repast Simphony includes a High Performance Computing extension (see Collier and North, 2013) that allows models to be distributed over grids of connected computers, but this advanced feature can only be leveraged by using the C++ language. As part of the design process, it will be worthwhile to consider how complex and computationally expensive the final model will be, and whether the additional difficulty in learning a more advanced tool will be offset by the advantages in performance and flexibility.

1.16.4.3 Evaluating a Model

As illustrated in Fig. 6, it is very unlikely that the model-building process ends once the model has been implemented. It is much more likely that insights into the model that are gained during the process of *evaluating* a complete model will cause the designer to repeatedly return to the initial model design to add refinements that require subsequent implementation. Far from being a burden, this process actually highlights one of the significant advantages of ABM over other methodologies. As the model is developed, the researcher has an opportunity to test their understanding of how the target system works. An ABM will rarely behave exactly as expected, so the model itself and our understanding of the phenomenon that it is modeling have a chance to *coevolve*.

It is nevertheless vital to properly evaluate models because, as the famous quote from Box (1979) suggests: "all models are wrong but some are useful." If models are to be useful as tools to explore the real-world, then they need to replicate the behavior of their target system to a certain level of accuracy. This degree to which models are able to do this is often termed their *validity*, that is, the extent to which the model is able to represent the system it is attempting to simulate (Casti, 1997). While perfection is neither possible nor desirable (a perfect model ceases to be a model at all), it is important to understand the levels of uncertainty in a simulation. However, robust evaluation is a step that is often overlooked or given minimal attention. There is no formal methodology for evaluating agent-based models, but the community has largely settled on a standard process that consists of *verification*, *calibration*, and *validation* (although naturally the terms differ across authors).

1.16.4.3.1 Verification

Broadly, verification refers to the process of ensuring that the model implementation corresponds to the model design. In other words, has the model been programmed correctly? This can be thought of as "internal validity" (Axelrod, 1997). One way to increase the reliability of the model is to make use of the techniques that computer programmers have developed. A range of techniques exist that can help to support the writing of accurate code and to provide mechanisms to test for errors (see Balci, 1996). Unit testing, for example, is a common approach, whereby every part of the codebase (the individual "units") is tested. A more rigorous, although probably more time-consuming approach, is docking (Axtell et al., 1996). Docking refers to the process of creating a second model separately from the first in order to ascertain whether similar results can be replicated from both. Ideally, the two models are created in different languages and by different developers.

1.16.4.3.2 Calibration

Having verified the model implementation (i.e., determining that the model implementation has accurately captured the design), it is possible to *calibrate* the model. In effect, calibration is the process of adjusting model parameters so that the behavior of the model closely matches some observed (often historical) conditions (O'Sullivan, 2004). This is also known as "fitting" the model to some observed data (Gilbert and Terna, 2000). Calibration is necessary because the theory and empirical evidence that were used to create the general structure of the model are usually insufficiently precise to allow for detailed parameterization. For a hypothetical example, consider an agent rule that determines the conditions under which an agent who is taking part in a marathon will give up and drop out of the race. Theory might suggest that the probability of dropping out ($P_{\text{drop out}}$) is influenced in part by levels of energy and in part to psychological motivation:

$$P_{\text{drop out}} = x_1 \times \text{energy} + x_2 \times \text{motivation}$$

While that theory might be reliable, it is insufficiently precise to tell us how important each of those factors are in the overall decision. Hence calibration is required to find the most appropriate values for x_1 and x_2. In other words, the rules that drive the behavior of the agents might be correct, but we might not have enough information to implement them precisely.

Calibration is actually performed by comparing the behavior of the agent-based model to some data that describe the real system. Typically, the approaches are either quantitative or qualitative. Quantitative calibration involves computing the difference between the simulation outputs to real data and calculating a "fitness" value (i.e., a number that represents the similarity between the two datasets). If comparable data are not directly available, it is common to use "stylized facts" (e.g., Heine et al., 2005). As an example, rather than comparing the routes taken by agents in a transport model to real data, one could assess the success of the model on how well it simulated the overall commute time (a very simplified representation of the route taken). Alternatively, qualitative calibration—also known as "face calibration" or "face validity" (Gravetter and Forzano, 2011)—consists of exploring the model results and using human intuition to assess its similarity to the real-world. With face calibration of spatial models, GIS and spatial data visualization are important components as the success of the calibration might rely on the quality of the maps used to compare the two datasets. These difficulties are discussed in more detail later.

1.16.4.3.3 Validation

Calibrating a model to real-world data runs the risk of *overfitting* the model to the data. A model that has been overfitted will not generalize well to contexts other than the one that it was calibrated on. Therefore, validation completes the process of evaluating a model by testing it on some new data. The aim of the validation is to demonstrate that the model is sufficiently accurate given the context of the system that it is attempting to simulate. If the model is able to reliably replicate real-world conditions that it has not been "fitted" to (i.e., calibrated on), then we can be reasonably confident that it can be applied to new scenarios and to explore potential futures. Typically the methods to assess the success of validation (i.e., model fitness) are the same as those used during the calibration stages. For interested readers, Axtell and Epstein (1994) offer guidelines for validating agent-based models depending on their purpose. The authors categorize these purposes on a scale ranging from models that portray a caricature of the agents' behavior to those that attain quantitative agreements with both emergent macro-structures as well as individual agent's micro-behavior. An ongoing problem, however, is how to obtain high-resolution data to support validation.

1.16.4.3.4 Difficulties in evaluating spatial models

It is important to stress that assessing how well an agent-based model represents the underlying system is usually extremely challenging. One of the reasons that it can be so difficult is because to properly evaluate a model it must be examined at multiple hierarchical levels. For example, in the segregation example presented in section "**What Is ABM?**", to properly evaluate the reliability of the model in comparison with real-world data, it would be necessary to look at more than just the overall degree of segregation. One might examine the decision process of the agents before and after moving, or compare the actual moves themselves to real data. Fortunately, frameworks are emerging to support the complicated process of validating complex models by examining model behavior at numerous hierarchical scales. POM (Grimm et al., 2005) is arguably the most well-known and widely cited example. POM advocates the comparison of numerous patterns produced by models and their counterparts in real (nonsimulated) data. Commonly in ABM, this involves analyzing model outcomes at multiple spatial and temporal scales. To further complicate matters, it can be very difficult to quantify the difference between two spatial patterns (i.e., modeled and observed), even if data are available. Face validation, as discussed earlier, is a common means of comparing spatial patterns, but one that is subjective (one person might see similar patterns where another would not). Instead, spatial statistics can be used to provide quantitative assessments of the similarity between simulated and observed data. For example, the Nearest Neighbor Index (Clark and Evans, 1954) and Ripley's K (Ripley, 1977) both quantify the degree of clustering in point datasets (for a comprehensive review of such statistics, the interested reader is directed to O'Sullivan and Unwin (2010)). Statistics that are not inherently spatial can also be applied if the data are aggregated to some boundary areas (e.g., administrative areas or a regular grid). Statistics such as R^2 and the standardized root mean square error (SRMSE) have been found to give reliable error assessments for spatial models (Knudsen and Fotheringham, 1986). A further advantage to performing validation using statistics, other than the quantitative rigor introduced, is that algorithms can be used to automatically parameterize models without the need for human intervention. Routines such as simulated annealing and genetic algorithms have been used to successfully parameterize complex agent-based models (e.g., Malleson et al., 2009).

The remaining hurdle to overcome in the evaluation of spatial agent-based models is that of data. As already noted, data are required at different scales in order to properly evaluate a complex model (Grimm et al., 2005). It is not sufficient to evaluate the model outcomes at an aggregate level in isolation; rather it would be preferable to have individual-level data that can be used to evaluate the behavior of *individual agents* as well (thus being confident that we are not only capturing the emergent macro-structures but also the individual agents' micro-behavior). Traditionally it has been very hard to find good-quality, high-resolution data for these purposes. However, the emergence of "big" data and the associated "datafication" of previous undocumented aspects of peoples' everyday lives (e.g., moods, thoughts, activities, feelings) through sources like social media (among others) have led to the proliferation of sensitive individual-level data (Mayer-Schönberger and Cukier, 2013) that have the potential to transform the quality of agent-based models. Section "**Challenges and Opportunities**" will discuss this emerging trend and the opportunities it offers agent-based modelers in more detail.

1.16.5 Integrating GIS and Space Into Agent-Based Models

Consideration of space is often integral to the success of agent-based models. For example, in the Schelling model presented in section "**What Is ABM?**", the agents' decision making is directly impacted by its neighbors. In the sense that if the agent is dissatisfied with its current location (based on the mix of neighbors) it can move to an empty cell, thus directly impacting the landscape. Considering how agents can react to each other and change their environment, we would argue that ABM has great relevance to many geographical problems (as discussed in sections "**The Rise of the (Automated) Machines**" and "**What Is ABM?**") and there has been growing interest in the integration of GIS and ABM (e.g., Benenson and Torrens, 2004; Gimblett, 2002; Heppenstall et al., 2012). This interest arises as it allows agent-based models to be related to actual geographical locations, thereby explicitly incorporating space into the model design. Furthermore, it allows modelers to think about how objects or agents and their aggregations interact and change in space and time (Batty, 2005). For GIS users, it provides the ability to model the emergence of phenomena through individual interactions of features within a GIS over time and space. This last point is a movement away from traditional focus of GIS where more attention was focused on spatial representation, often ignoring temporal representations (Peuquet, 2002). Moreover, from a understanding of geographical systems perspective, this linkage is highly appealing in the sense that while GIS provides us with the ability to monitor the world, it provides no mechanism to discover new decision-making frameworks such as why people have moved to a new areas (Robinson et al., 2007). Through the integration of GIS and ABM we can capture both.

The simplest way to visualize the integration of geographical data and ABM is by taking the view most GIS's do of the world, as shown in **Fig. 7**. The complexity of the world is abstracted away and represented as a series of layers (such as the physical environment, the built environment). These layers form the environment for our artificial world for which the agents inhabit; they can act as boundaries for our simulations, or fixed layers such as roads provide a means for agents to move from A to B, or houses provide them with a place to live. Aggregate spatial data also allow for model validation (as discussed in section "**Evaluating a Model**"): for example, are the land-use patterns we see emerging from a model of urban growth matching that of reality? If they do, it provides us with an independent test of the micro-level processes encoded within the model.

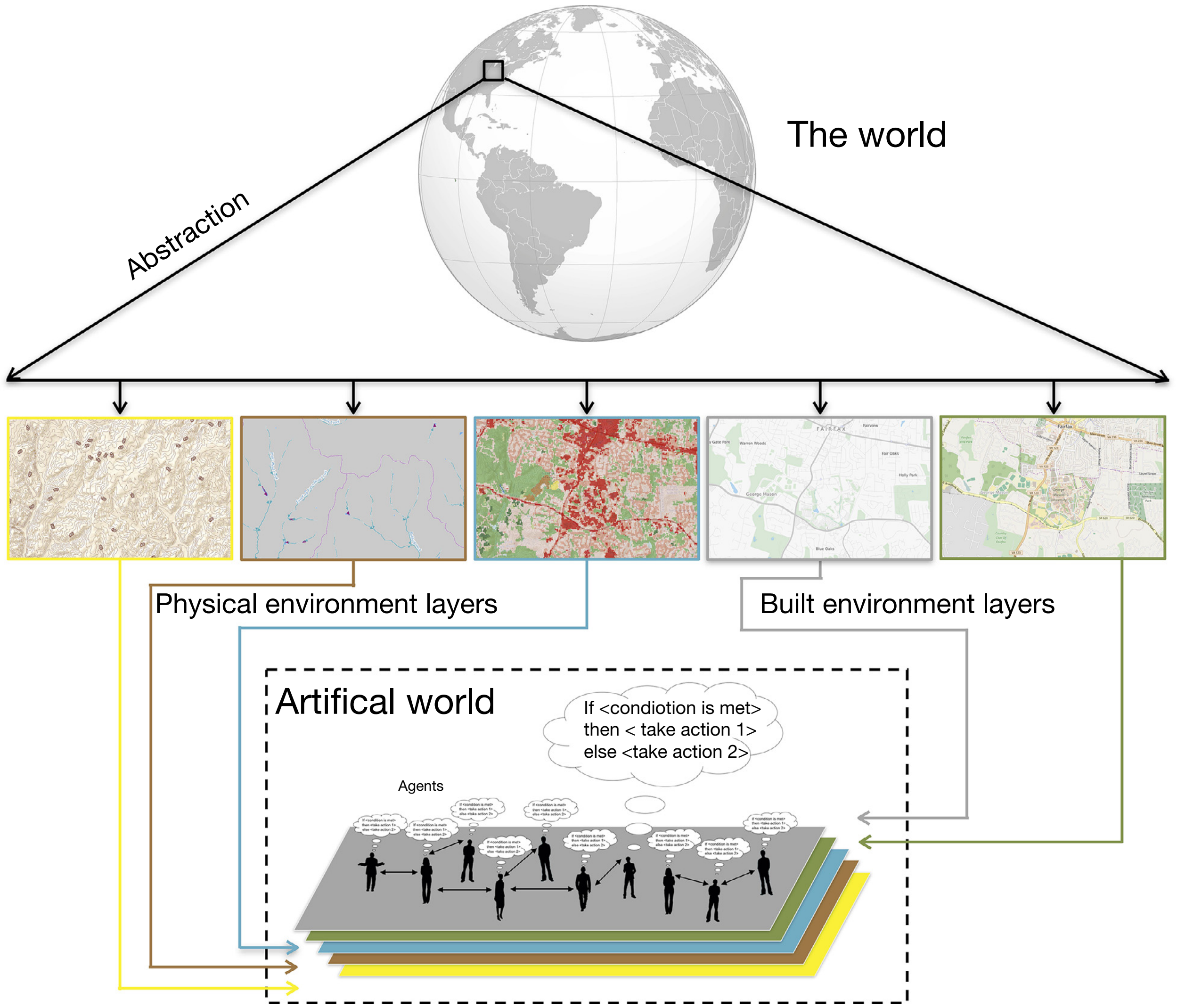

Fig. 7 Abstracting from the "real" world into a series of layers to be used in the artificial world for which to base the agent-based model upon.

1.16.5.1 Coupling and Embedding GIS and Agent-Based Models

The question faced by many modelers' is how to go about integrating geographical data into models as many traditional GIS platforms are not capable of representing continuous data over time and space. This has led to modeler's either linking (coupling) GIS and ABM or embedding GIS into the ABM or vice versa (see Crooks and Castle, 2012 for a detailed discussion). Coupling can be broadly defined as the linkage of two stand-alone systems by data transfer. Westervelt (2002) identifies three coupling approaches (loose, moderate, and tight) with respect to GIS and ABM. Loose coupling involves the asynchronous operation of functions within each system, with data exchanged between systems in the form of files. For example, the GIS might be used to prepare inputs, which are then passed to the modeling system, where after execution the results of the model are returned to the GIS for display and analysis (e.g., Crooks, 2010). This approach requires the GIS and modeling system to understand the same data format (e.g., ESRI shapefiles). At the other extreme is tight coupling which can be characterized by the simultaneous operation of systems allowing direct intersystem communication during the programme execution (e.g., Leavesley et al., 1996; Benenson et al., 2005). For example, standards such as Microsoft's COM and .NET allow a single script to invoke commands from both systems (Ungerer and Goodchild, 2002). In the middle is moderate coupling, which essentially encapsulates techniques between loose and tight coupling. For example, remote procedures that call and share database access link between the GIS and modeling system, allowing indirect communication between the systems (e.g., Harper et al., 2002). For a review of the pros and cons of different coupling approaches, the reader is referred to Westervelt (2002) for a review.

Traditionally coupling has often been the preferred approach for linking GIS and modeling systems. However, this has tended to result in very specialized and isolated solutions, which have prevented the standardization of general and generic linkage. An alternative to coupling is to embed or to integrate the required functionality of either the GIS or modeling system within the dominant system using its underlying programming language (Maguire, 2005). The final system is either referred to as GIS-centric or modeling-centric depending on which system is dominant. In both instances, the GIS tools or modeling capabilities can be executed by calling functions from the dominant system, usually through a graphical user interface (GUI). Compared to coupling, an embedded or integrated system will appear seamless to a user (Maguire, 1995).

Interest in modeling-centric systems has increased considerably over recent years, predominately due to the development of modeling toolkits with scripting capabilities that do not require advanced computer-programming skills (Castle and Crooks, 2006; Gilbert and Bankes, 2002). Often the modeling toolkit can access GIS functions, such as data management and visualization capabilities, from a GIS software library. For example, the MASON (Multi Agent Simulation Of Neighbourhood) toolkit (see section "**ABM Toolkits**") exploits functions from GeoTools (a Java GIS software library) for importing and exporting data, Java Topology Suite (JTS) for data manipulation, and its own GUI for visualization. The toolkit itself maintains the agents and environment (i.e., their attributes), using identity relationships for communication between the different systems. Functions available from GIS software libraries reduce the development time of a model, and are likely to be more efficient because they have been developed over many years with attention to efficiency. Additionally, the use of standard GIS tools for spatial analysis improves functional transparency of a model, as it makes use of well-known and understood algorithms (Castle and Crooks, 2006).

Conversely, the GIS-centric approach is an attractive alternative; not least because the large user-base of some GIS expands the potential user-base for the final model. Analogous to the modeling-centric approach, GIS-centric integration can be carried out using software libraries of modeling functions accessed through the GIS interface. While there are many examples of modeling systems integrated within commercial GIS, including: the Consequences Assessment Tool Set (Kaul et al., 2004) system which was designed for emergency response planning; the Hazard Prediction and Assessment Capability (DTRA, 2001) system, for predicting the effect of hazardous material releases into the atmosphere; the NatureServe Vista (2016) system, for land-use and conservation planners. There are few GIS-centric implementations from an ABM perspective, one such example is Agent Analyst for ArcGIS (see Johnston, 2013).

1.16.5.2 ABM Toolkits

Traditionally the building of agent-based models required their development from scratch. However, over the years several ABM toolkits have been developed which allow for more ease with respect to the development of the agent-based model. Specifically, it has been argued that toolkits reduce the burden modelers face programming parts of a simulation that are not content-specific (e.g., GUI, data import–export, visualization/display of the model). Toolkits also increase the reliability and efficiency of the model, because complex parts have often been created and optimized by professional developers, as standardized modeling functions (Castle and Crooks, 2006).

However, there may be limitations of using toolkits to develop agent-based models, for example: in some instances a substantial amount of effort is required to understand how to design and implement a model in some toolkits; the programming code of demonstration models or models produced by other researchers can be difficult to understand, poorly documented, or apply to another purpose; a modeler will have to learn or already have an understanding of the programming language required to use the toolkit (e.g., Java, C); and finally the desired/required functionality may not be present, although additional tools might be available from the user community or from other software libraries. Benenson et al. (2005) also note that toolkit users are accompanied by the fear of discovering that a particular function cannot be used, will conflict, or is incompatible with another part of the model late in the development process.

In this section we present an overview of a selection of open-source ABM toolkits that have the capability to process spatial (GIS) data as shown in **Table 2**. We list the projects website in order for readers to find out more about the current state of development of each toolkit. Our rationale for only choosing open source is that their source code is published and made available to the public, enabling anyone to copy, modify, and redistribute the system without paying royalties or fees. A key advantage of open-source toolkits relates to the transparency of their inner workings. The user can explore the source code, permitting the modification, extension, and correction of the system if necessary, thus relaxing the fear of the unknown. This is particularly useful for verifying and validating a model (see Crooks et al., 2008). Readers interested in other platforms or guidelines for choosing an ABM toolkit are referred to reviews by Castle and Crooks (2006), Kravari and Bassiliades (2015), Nikolai and Madey (2009), Railsback et al. (2006), Robertson (2005) and for a comprehensive list of other ABM toolkits are referred to Wikipedia (https://en.wikipedia.org/wiki/Comparison_of_agent-based_modeling_software).

Swarm could be classed as the original ABM toolkit designed specifically for the development of simulations of complex adaptive systems (Swarm, 2016). Inspired by artificial life, Swarm was designed to study biological systems; attempting to infer mechanisms observable in biological phenomena (Minar et al., 1996). In addition to modeling biological systems such as fish (e.g., Railsback and Harvey, 2002), Swarm has been used to develop models for anthropology, computer science, ecological, economic, geographical, and political science purposes (e.g., Deadman and Schlager, 2002; Johnson, 2002; Lim et al., 2002). Useful examples of spatially explicit models include: the simulation of pedestrians in the urban centers (Haklay et al., 2001); and the examination of crowd congestion at London's Notting Hill carnival (Batty et al., 2003).

MASON is developed by the Evolutionary Computation Laboratory (ECLab) and the Centre for Social Complexity at George Mason University (see Luke et al., 2005). Core functionality includes dynamically charting (e.g., histograms, line graphs) and model output during a simulation. It has a strong support for using GeoMASON (Sullivan et al., 2010) which allows GIS vector and Raster data to be imported/exported. MASON has a comprehensive set of technical documents and well-commented Javadocs. MASONs how-to documentation, demonstration models, and several publications detailing the implementation and/or application of

Table 2 A selection of open-source ABM toolkits for creating geographical explicit models

	Swarm	*MASON*	*Repast*	*NetLogo*	*GAMA*
Developers	Santa Fe Institute/SWARM Development Group, USA	Evolutionary Computation Laboratory and Center for Social Complexity, George Mason University, USA	University of Chicago, Department of Social Science Research Computing and Argonne National Laboratory, USA	Centre for Connected Learning and Computer-Based Modelling, Northwestern University, USA	UMMISCO, France
Date of inception	1996	2003	2000	1999	2007
Website	http://www.swarm.org/	http://cs.gmu.edu/∼eclab/projects/mason	https://repast.github.io/	https://ccl.northwestern.edu/netlogo/	http://gama-platform.org/
Implementation language(s)	Objective-C/Java	Java	Java, Microsoft.Net Python, Groovy, ReLogo	Proprietary scripting	Proprietary scripting: GAMA Modeling Language
Required programming experience	Strong	Strong	Medium to strong	Basic	Basic to medium
Integrated GIS functionality	Yes (e.g., Kenge GIS library for Raster data, see Box, 2001)	Yes	Yes	Yes	Yes
Integrated charting/ graphing/ statistics	Yes (e.g., R- and S-plus statistical packages)	Yes (e.g., wrappers for JFreeChart)	Yes	Yes	Yes
Availability of demonstration models	Yes	Yes	Yes	Yes	Yes
Tutorials/how-to documentation	http://www.swarm.org/wiki/Swarm_main_page	http://cs.gmu.edu/∼eclab/projects/mason/docs/Also Luke, 2015	https://repast.github.io/docs.html	https://ccl.northwestern.edu/netlogo/resources.shtml also Wilensky and Rand, 2015	http://gama-platform.org/tutorials
Additional information	Minar et al. (1996)	D-MASON: www.dmason.org/ GeoMASON: http://cs.gmu.edu/∼eclab/projects/mason/extensions/geomason/	Useful weblog: http://crimesim.blogspot.com/ Agent Analyst: http://resources.arcgis.com/en/help/agent-analyst/	NetLogo-R Extension: http://r-ext.sourceforge.net/ Selection of GIS examples: http://www.gisagents.org/search/label/NetLogo	GAMA GitHub page https://github.com/gama-platform

Adapted and extended from Parker, D. C., Berger, T. and Manson, S. M. (2001). *Proceedings of an International Workshop on Agent-Based Models of Land-Use and Land-Cover Change*, Irvine, CA; Castle, C. J. E. and Crooks, A. T. (2006). Principles and concepts of agent-based modelling for developing geospatial simulations. Centre for Advanced Spatial Analysis, University College London, Working paper 110, London.

MASON are available for a prospective modeler to evaluate the system further (see MASON, 2016). Examples of spatially explicit models utilizing MASON's GIS functionally are shown in **Fig. 8**. Spatial applications of MASON include exploring disease spread (Crooks and Hailegiorgis, 2014), evacuation (Wise, 2014), conflict between herdsmen and farmers in East Africa (Kennedy et al., 2010), and movement across national borders (Łatek et al., 2012) to name but a few. More recently, a distributed version of MASON (D-MASON; Cordasco et al., 2013) was created which allows MASON models to be run over cluster and cloud-computing architectures.

Repast (Recursive Porous Agent Simulation Toolkit) was originally developed at the University of Chicago, and is currently maintained by Argonne National Laboratory. Earlier incarnations of Repast catered for the implementation of models in three programming languages: Python (RepastPy); Java (RepastJ); and Microsoft.Net (Repast.Net) (see Collier and North, 2004; North et al., 2006; Vos and North, 2004 for more details and for a review of their GIS functionality see Crooks, 2007). These earlier versions have been superseded by Repast Simphony (North et al., 2013), which provides all the core functionality of previous versions but allows models to be developed in several ways including the ReLogo (a dialect of Logo; Ozik et al., 2013), point-and-click statecharts (Ozik et al., 2015), Groovy, or Java.

The Repast development team have provided a series of articles regarding Repast Simphony. The architecture and core functionality are introduced by North et al. (2005a), and the development environment is discussed by Howe et al. (2006). The storage, display, and behavior/interaction of agents, as well as features for data analysis (i.e., via the integration of the R statistics package) and presentation of models within Repast Simphony are outlined by North et al. (2005b). In relation to the integration of GIS functionality, the reader is referred to the tutorials by Malleson (2012) which demonstrates how to create a virtual city via

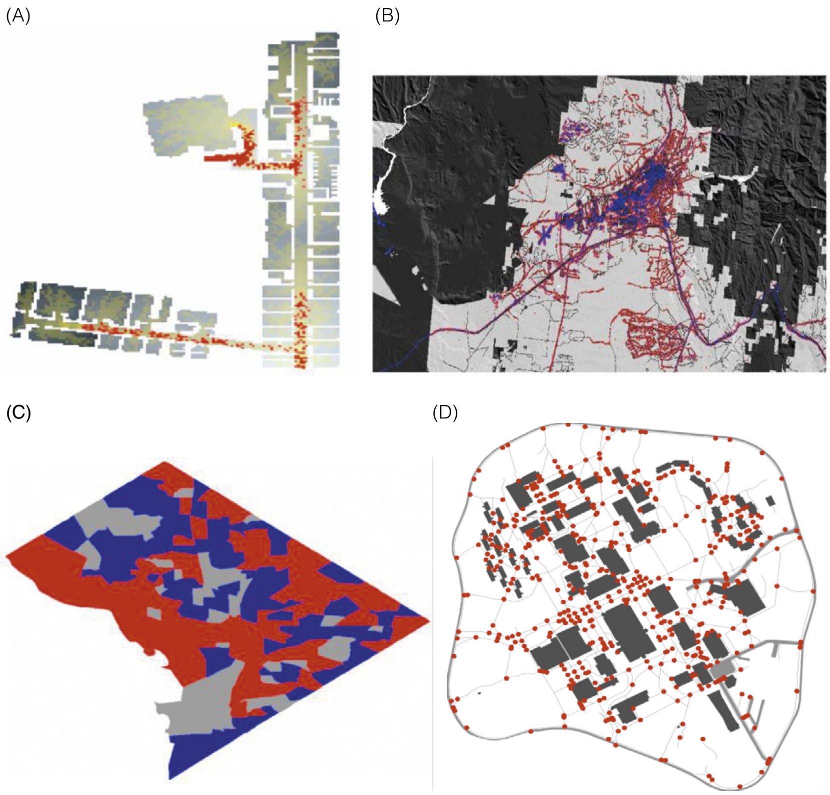

Fig. 8 A selection of MASON spatial models (A): agents (*red*) exiting a building based on raster data and the resulting trails (*yellow*). (B) An urban growth model where *red areas* represent new developments. (C) A Schelling-type model using census areas in Washington, DC as its spatial environment. (D) Agents (*red circles*) moving along on sidewalks (*gray lines*).

the importation of shapefiles, create agents, and then move the agents around a road network (this tutorial was used for the creation of Fig. 9A). Furthermore, within Repast Simphony it is possible to embed spatially explicit agent-based models directly into a 3D GIS display. For this Repast Simphony provides methods to directly visualize agent-based models to NASA's virtual globe—World Wind. This interactive 3D GIS display allows one to visualize agents with satellite imagery, elevated terrain, and other scientific datasets as shown in Fig. 9B. Repast Simphony also supports the importation of NetLogo models into the Repast framework via Repast Simphony (Ozik et al., 2013; North et al., 2013). Such functionality aims to allow for rapid prototyping of agent-based models by first building simple agent-based models in NetLogo and once satisfied with its basic functionality migrate and extend them in Repast Simphony (for a comparison of NetLogo and ReLogo see Lytinen and Railsback, 2012). Repast Simphony

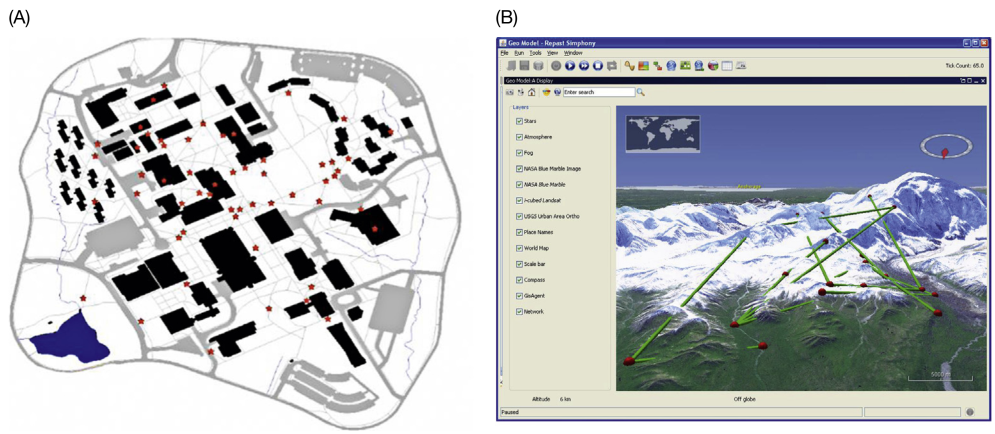

Fig. 9 Examples of vector agent-based models in Simphony. (A) Agents (*red stars*) moving along on sidewalks (*gray lines*). (B) An agent-based model overlaid on NASA world wind. *Source*: Repast. (2016). Recursive porous agent simulation toolkit. Available at http://repast.sourceforge.net/ (accessed on 7 Oct. 2016).

also supports high-performance distributed computing via Repast for High Performance Computing (Repast HPC, see Collier and North, 2013) and has extension called Agent Analyst that allows users to create, edit, and run Repast models from within ArcGIS (see Johnston, 2013).

Useful examples of spatially explicit models created using Repast include the studying of segregation, and residential and firm location (Crooks, 2006), residential dynamics (Jackson et al., 2008), urban regeneration (Jordan et al., 2014), crime (Malleson et al., 2010), land-use change (Deadman et al., 2004), pedestrian evacuation (Castle, 2007), and disaster management (Mysore et al., 2006).

NetLogo was developed at the Centre for Connected Learning and Computer-Based Modeling at Northwestern University and uses a dialect of the Logo language to create agent-based models. NetLogo has been used to develop applications in disciplines varying from biology and physics to the social sciences (see Wilensky and Rand, 2015). It has extensive how-to documentation/tutorials and demonstration models which are available from its website, and functionality can be extended through application programming interfaces (APIs). For example, NetLogo also has an R extension allowing for more greater statistical analysis of model structure and dynamics (Thiele and Grimm, 2010). Another interesting feature of NetLogo is that it allows for multilevel modeling (via LevelSpace) by being able to connect several models together. For example, if one had a model of population growth, another on food projection, and another on weather, you can explore how these three systems impact each other (i.e., how bad weather impacts food production and how this population growth). Moreover, models developed in NetLogo can also be run on the web via NetLogoWeb. NetLogo is simple to use and it is possible to import both raster (in the form of .asc files) and vector data (shapefiles). This ability opens up a range of possibilities for the easy creation of spatial agent-based models as shown in **Fig. 10**; for example, for the studying of basic concepts of water flow and surface erosion as shown in **Fig. 10A**. A raster file of surface elevation is loaded into a NetLogo model where the agents follow the surface to lower

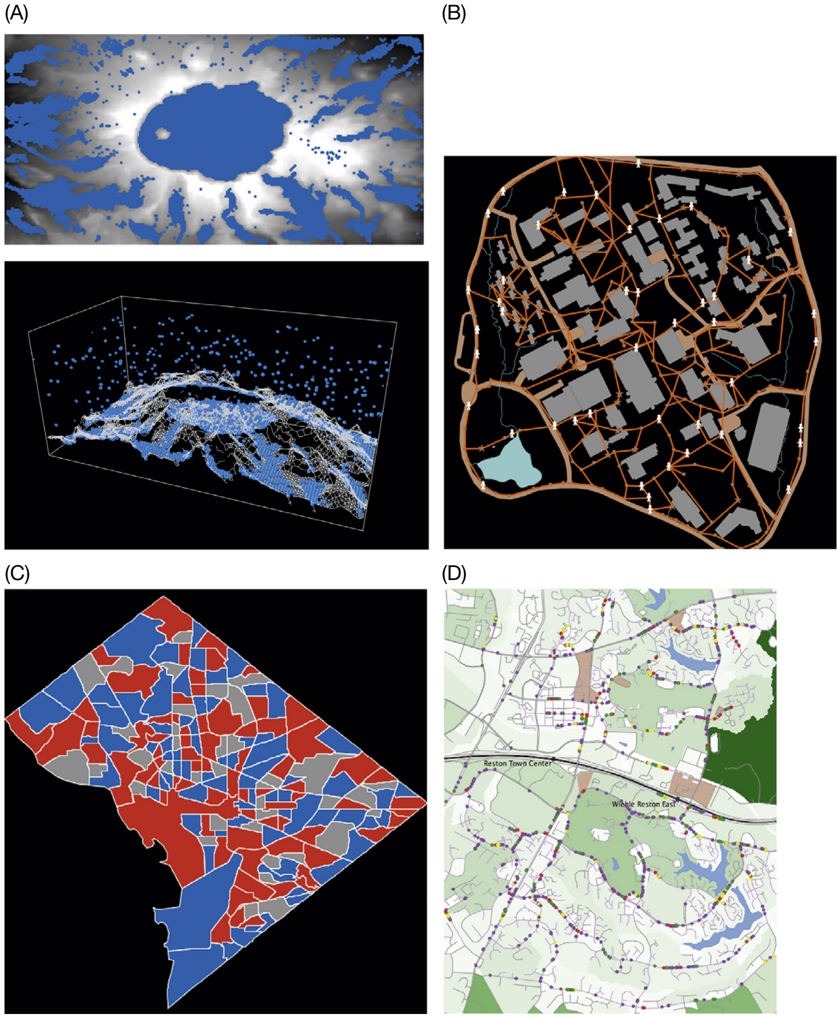

Fig. 10 A selection of geographically explicit agent-based models utilizing NetLogo. (A) Rainfall where rain (*blue*) falls and flows to a lower elevation based on a digital elevation model captured in 2D and 3D. (B) Agents (*white*) moving along on sidewalks (*orange*). (C) The Schelling-type model using census areas in Washington, DC as their spatial environment. (D) Commuting along a road network.

elevations. Such functionality potentially lowers the barrier between linking agent-based models and GIS to none expert programmers. For example, the gradient example presented earlier could be used to model process that relies on cost surfaces such as used in pedestrian moment models (see Crooks et al., 2015a). NetLogo models can also be viewed in a 3D environment and 3D surfaces can also be incorporated in such models as shown in the bottom of **Fig. 10A**. Vector data can also be imported and used as a foundation of models such as polylines can act as sidewalks or roads for agents to navigate the urban environments (**Fig. 10B** and **D**), and polygons can act as cells for a segregation type of model (**Fig. 10C**). Useful examples of spatially explicit models created using NetLogo include the study of gentrification (Torrens and Nara, 2007), residential housing demand (Fontaine and Rounsevell, 2009) and the reimplementation of Axtell et al.'s (2002) artificial Anasazi model by Janssen (2009).

GAMA (GIS Agent-based Modeling Architecture): is the only platform we review here that was specifically designed for the development of spatially explicit models ranging from hundreds to millions of agents (Taillandier et al., 2016). It was developed by several teams under the direction of UMMISCO (Unit for Mathematical and Computer Modelling of Complex Systems), France (Amouroux et al., 2007). Its intention was and still is to allow for the simple creation of models (akin to NetLogo) but with the ability to carry out experiments and simulations as in MASON and Repast (Grignard et al., 2013). At its time of inception, it was noted that existing toolkits had several weaknesses with respect to creating geographically explicit models. For example, complex programming for new modelers when using Swarm, or no GIS support in MASON and the inability of NetLogo to have complex models which GAMA aimed at overcoming (Amouroux et al., 2007).

GAMA has its own domain-specific language GAML (*GA*ma *M*odeling *L*anguage) which is coded in Java and its application is based on the rich client platform (RCP) architecture provided by Eclipse. It allows for the importation of shapefiles, OpenStreetMap data along with grid and 3D files (e.g., .3ds file format) which allows for the creation of multilevel highly visual and geographically explicit models in 2D and 3D as shown in **Fig. 11**. Similar to other platforms it has built in charting and statistical functions including the Fuzzy−Kappa simulation (van Vliet et al., 2013) and an integrated BDI cognitive architecture that others can use if they wish (Caillou et al., 2015). For example, spatially explicit applications utilizing GAMA include farming (Taillandier et al., 2012), 2D and 3D pedestrian evacuation (Anh et al., 2011; Macatulad and Blanco, 2014), traffic simulation (Taillandier, 2014), urban growth (Taillandier et al., 2016), land-use planning (Caillou et al., 2015), and river sedimentation (Grignard et al., 2015).

1.16.5.3 Example Applications

Agent-based models have been developed to study a wide range of phenomena from a number of academic disciplines (Macal, 2016). These range from archeological reconstruction of ancient civilizations (Axtell et al., 2002); understanding theories of political identity and stability (Cioffi-Revilla and Rouleau, 2010); exploring the processes that lead to state formation (Cederman, 2001); biological models of infectious diseases (Eidelson and Lustick, 2004); growth of bacteria colonies (Krzysztof et al., 2005); stock trading (Carrella, 2014) labor market dynamics (Guerrero and Axtell, 2011); tax compliance (Bloomquist, 2011); housing markets (Geanakoplos et al., 2012); and voting behaviors in elections (Laver and Sergenti, 2012) to name but a few.

From a geographical systems perspective, agent-based models have been applied to a wide range of phenomena, some have been highlighted earlier but these range from the micromovement of pedestrians over seconds and hours (e.g., Torrens, 2014) to the rise of city systems over centuries (e.g., Pumain, 2012) and nearly everything in-between. It is impossible to cover all in detail but **Table 3** gives a list of representative examples of agent-based models that use GIS to explore problems relate to geographical systems. As can be seen one question that preoccupies researchers is "how to select the most representative scale for an application in terms of agents (entities), spatial and temporal scales?" Fortunately, the underlying rationale for using ABMs is the notion of complexity, which focuses on a "bottom-up" approach to modeling geographical systems and provides a ready solution with the emphasis on representing the smallest individual unit of interest. The examples in **Table 3** present a range of agent representation from individuals, households to entire cities, or institutions. The choice of agents, spatial scale, and temporal scale depends on the problem being investigated (Heppenstall et al., 2016). Furthermore, in section "**Making Agents More Human**" we noted that one of the hallmarks of ABM is its ability to capture and model human behavior; therefore we classified how the selected models represent behavior in two ways; either as a mathematical approach or through the use of cognitive frameworks.

1.16.6 Challenges and Opportunities

The greatest strength of ABM is its ability to model complex social phenomena. The focus on the *agent* as the fundamental driver of system-wide behavior allows researchers to take important steps toward understanding what the consequences of individual behavior, and the interactions between individuals, are on geographical systems. Section "**Example Applications**" highlighted the sheer diversity of applications that are abundant in the literature that seek to replicate the main processes and drivers of geographical systems from the micro to macro scale. While it is clear that significant progress has been made in simulating systems from the bottom-up, several key challenges remain that researchers need to address. Within this section, we will outline these challenges and the opportunities that meeting these will create.

ABM advocates an understanding of social phenomena through simulation at the individual level. By creating heterogeneous individuals who can interact with other individuals and the environment, we can track the emergence of new patterns or trends.

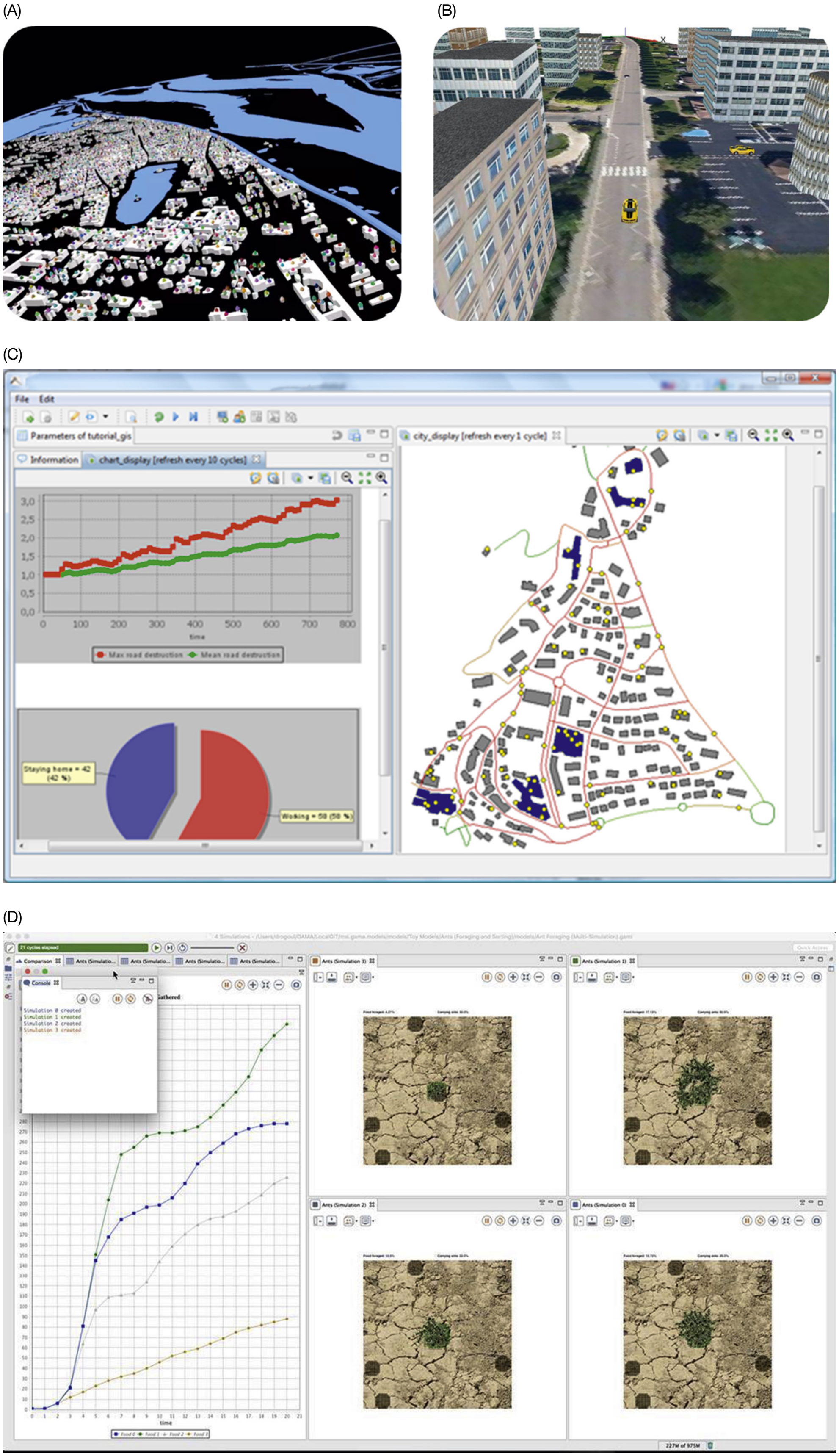

Fig. 11 GAMA platform: advanced visualization of simulations (A and B). (C) Built in charting and functions. (D) User interface. *Source*: GAMA. (2016). GAMA modeling and simulation development environment. Available at http://gama-platform.org/ (accessed on 20 Oct. 2016).

Table 3 A selection of the studies utilizing GIS and ABM

Author	*Application*	*Entity*	*Behavior*	*Spatial scale*	*Temporal scale*
Batty et al. (2003)	Public event	Individuals	Mathematical	Neighborhood	Seconds
Torrens and McDaniel (2013)	Riots	Individuals	Mathematical	Neighborhood	Seconds
Crooks et al. (2015a)	Indoor movement	Individuals	Mathematical	Indoor scene	Seconds
Crooks and Hailegiorgis (2014)	Disease propagation	Individuals	Mathematical	City	Minutes
Eubank et al. (2004)	Disease propagation and urban traffic	Individuals	Mathematical	City	Seconds
Malleson et al. (2013)	Crime	Individuals	Cognitive framework	Neighborhood	Minutes
Groff (2007)	Crime	Individuals	Mathematical	City	Hours
Manley et al. (2014)	Traffic	Individuals	Mathematical	City center	Seconds
Dawson et al. (2011)	Flooding	Individuals	Mathematical	Town	Minutes
Heppenstall et al. (2006)	Retail	Individuals	Mathematical	City	Days
Benenson et al. (2002)	Residential location	Individuals	Mathematical	Neighborhood	Years
Augustijn-Beckers et al. (2011)	Informal settlement growth	Households	Mathematical	Neighborhood	Days
Jordan et al. (2014)	Regeneration	Households	Mathematical	Neighborhood	Years
Haase et al. (2010)	Urban shrinkage	Households	Mathematical	City	Years
Xie and Fan (2014)	Urban growth	Institutions and developers	Mathematical	Region	Years
Pumain (2012)	City systems	City	Mathematical	Countries and continents	Years

Adapted from Heppenstall, A., Malleson, N. and Crooks, A. T. (2016). "Space, the final frontier": How good are agent-based models at simulating individuals and space in cities? *Systems* 4(1): 9. Available at http://www.mdpi.com/2079-8954/4/1/9/html.

While this is a tantalizing prospect for researchers, it is accompanied by a new set of problems. Let us consider how we might, for example, simulate the behavior of individuals evacuating a building in an emergency. How the individuals would react in this situation is highly dependent on their individual attributes. Their behavior is a product of their attributes and, in this case, explicitly influenced by their local environment. While we are approaching the point where we can obtain and build this information into our agents, we need a corresponding amount of data to calibrate and validate the behavior. As Heppenstall et al. (2016) note, it is ironic that the disaggregation of data down to the individual level to give better representation through heterogeneity has meant that it is near impossible (at present) to rigorously calibrate and validate our models. However, the recent proliferation of "big" data offers a potential resolution to this problem in the near future. While the abundance of data will contribute to solving this issue, how we extract value and make sense of these new forms of data presents a considerable challenge. These issues are revisited here.

O'Sullivan et al. (2012) speculate that social systems are potentially the product of thousands of individual's decisions—it therefore follows that researchers need to include behavioral frameworks (see section "**Making Agents More Human**") that can manage more complex behaviors to capture these decisions. Many of the behaviors in the examples in section "**Example Applications**" operate through rule-based systems that are more closely related to mathematics than psychology. While this is entirely appropriate for some applications, human behavior cannot be distilled down into formulaic rules. Human decisions are made on the basis of incomplete or assumed knowledge with decisions which can be both spontaneous and irrational. To grasp some of this complexity, there needs to a more explicit link between ABM and behavioral frameworks. Frameworks such as BDI (Bratman et al., 1988) are a popular choice among modelers (e.g., Müller, 1998; Rao and Georgeff, 1995; Taylor et al., 2004), but are limited by assumptions of rational decision making that can be difficult to justify as people rarely meet the requirements of rational choice models (Axelrod, 1997). The work of Malleson et al. (2012) and Pires and Crooks (2016) shows how alternative frameworks such as PECS can be successfully integrated with agent-based models.

While we can begin to create more complex agent-based models, quantitative geography has not yet focused on the development of methods for measuring and analyzing individual units as part of a massively interactive, dynamic, and nonlinear system (Batty and Torrens, 2005; Torrens, 2010). This has precipitated the criticism of agent-based models as "toy models," that is, an absence of robust quantitative schemes to allow ABM to be held up to account against real-world systems.

This is an area where "big" data sources could offer new avenues for multiscale calibration and validation of agent-based models. Putting aside the difficulties associated with quantifying the similarity between spatial patterns (as discussed in section "**Evaluating a Model**"), the aggregate analysis of model results is often relatively unproblematic. But for patterns at higher spatiotemporal resolutions, assessing the reliability of model results can be extremely difficult when appropriate data are less forthcoming. For example, when modeling pedestrian movement, it would be desirable to compare the movements of individual-simulated agents to those of individual real people, rather than just the aggregate model outcomes (e.g., crowd densities, flow directions). This is where the emergence of "big" data, and associated developments around "smart cities," are particularly relevant. Data about individuals and the environment are being created at an unprecedented rate. Sources such as mobile phone call data records (Diao et al., 2016), public transport smart cards (Batty et al., 2013), vehicle traffic counters (Bond and Kanaan, 2015), the use of loyalty cards or credit cards, and social media contributions such as Twitter or FourSquare (Croitoru et al., 2013; Malleson and Andresen, 2015) can potentially reveal a wealth of information about individual behavior or actions. Additionally, unlike traditional sources that are largely static and often somewhat out of date—the most recent UK and US censuses were conducted in 2011 and 2010, respectively—"big" data are often generated in *real time*. Rather than being calibrated using historical data and then used to make future predictions in the absence of any new information, agent-based models could be calibrated *in real time* as new data emerge which will reduce the uncertainty in model predictions. This provides a substantial opportunity for ABM as a means of producing short-term, high-quality, local analyses and forecasts that can inform agile and responsive policy-making. This is particularly relevant for models that have been coupled to GIS, as these are often concerned with estimating future real-system states rather than exploring theory in hypothetical contexts. However, there has been relatively little work toward sound methodologies that support the incorporation of data into agent-based models dynamically. Methods to perform *dynamic data assimilation* that are used regularly in fields such as meteorology (Kalnay, 2003) have only been attempted for the most rudimentary of agent-based models (Ward et al., 2016).

Another significant challenge for the use of big data that must be overcome before they can be used to inform agent-based models relates to bias. Considering social media, for example, not only do a small number of individuals often contribute substantially more than all others, but the presence of the "digital divide" (Yu, 2006) means that some groups are much less likely to contribute to these emerging digital data streams than others. Models that are predicated on "big" data, therefore, might disregard the groups of people who by choice or circumstance do not leave a digital footprint. Any insight from these sources must therefore be taken in the context of the inherent biases and steps should be taken to understand the subsequent inaccuracies even if nothing can be done to completely remove them. There are also related ethical implications, with a major concern that the data might be predicated on relatively weak consent. For example, an individual might sign a contract or tick a box that gives permission for the (re)use of their data, but it is not always clear how *informed* the person actually is. In most cases it is extremely unlikely that someone is fully aware of the terms that they are agreeing to. For example, the Apple iTunes UK Terms and Conditions contained almost 7000 words (as of 13 Sep. 2016). This lack of informed consent offers some fundamental challenges to traditional ethical frameworks that usually rely on explicit (often documented) consent. Even if consent is properly informed, then some individuals might still be unaware of size and thoroughness of the digital footprint that they are creating. Fortunately, research institutions typically adhere to comprehensive ethical standards and frameworks. It is therefore up to these institutions to demonstrate that the data can be: stored securely; treated sensitively and ethically; and produce outcomes that are ultimately for social good.

1.16.7 Conclusion

ABM is rapidly establishing itself as the defacto tool to simulate the processes and drivers in geographical systems. It offers the tantalizing possibility of creating new insights and knowledge about how geographical systems have evolved to their current state and how they might develop in the future. A large part of ABM's popularity is down to the natural metaphor that agents offer for modeling individuals. This chimes with current geographical thinking as embodied by Batty (2013) who describes cities as being the product of hundreds of individual interactions occurring on dynamic networks, and O'Sullivan et al. (2012) who hypothesized that social systems are the product of potentially infinite numbers of human decisions. While many of the applications within this article have focused on human to human agent interactions, there is an increasing focus on understanding the outcomes of human behavior with environmental interactions. Section "**Example Applications**" provided examples of coupled human and natural systems (CHANS) that highlight the importance and benefit of simulating the human link to land use.

What is noticeable from recent applications of ABM is the increase in complexity (richness and detail) of the agents; a factor made possible through new data sources and increased computational power. This increase in detail at the individual level is the beginning of a step-change in social simulation modeling with researchers being able to create realistic systems driven by the individual. While there has always been "resistance" to the notion that social scientists should search for some "atomic element or unit" of representation that characterizes the geography of a place (Batty, 2012), the shift from aggregate to individual places agents as a clear contender to fulfill the role of "atom" in social simulation modeling. However, there are a number of methodological challenges that need to be addressed if ABM is to be taken up as the "atomic unit" in social simulation and be recognized as a powerful tool for policy modeling in key societal issues.

Evaluation of ABMs has been identified by numerous commentators as one of the most critical issues yet to be resolved in ABM (Angus and Hassani-Mahmooei, 2015; Axelrod, 1997; Crooks et al., 2008; Lee et al., 2015; Ngo and See, 2012; Takadama et al., 2008). While developments in ABM, such as ODD (Grimm et al., 2006) and empirical grounding of ABM mechanisms and agent attributes (Robinson et al., 2007; Smajgl et al., 2011; Windrum et al., 2007), have improved transparency and replicability in models, the massive diversity in outputs produced by micro-level interactions presents a significant challenge in distilling the most relevant and interesting results from a nearly endless sea of output data. ABM outputs demand a comprehensive exploration of the model behavior and model output that is just not realized at present (Angus and Hassani-Mahmooei, 2015) and presents a significant challenge for the researcher. As a result, agent-based models remain poorly calibrated and validated with researchers not fully grasping the importance of uncertainty associated with their models (Crooks et al., 2015b; Edmonds and Moss, 2004; Moss, 2008; Takadama et al., 2008). Sensitivity tests are largely absent from ABM and outputs are never associated with a confidence level. If these models are to achieve the credibility associated with global change models in the natural sciences, and thus be taken up in policy decision making, rigorous work is urgently needed in this area.

Big data will only increase in volume, variety, and veracity in the future—harnessing useable information and embedding with model simulations to aid policy implementation is key: a factor that has been recognized by national governments (Yiu, 2012). However, the appeal of big data presents as many risks as opportunities for researchers; for example, caution needs to be exercised to ensure that research is driven by the problem (and variables of interest) rather than data availability. While big data presents obvious opportunities for increasing the number and types of application in ABM, there is also the real possibility that the extant ABM deficiencies will become more acute as more people begin to (mis)use big data in such models. Key work is needed now to rigorously test big data led models to ensure that those that make it into the decision-making arena are credible. This will ensure that the marriage of big data and ABM presents a unique opportunity to address important societal issues.

While these challenges are substantial, not addressing them will lead to ABM eventually being discredited as a tool that can deliver real value both in the academic arena and in the public and private sectors. Meeting these challenges will unlock the potential of ABM, allowing new knowledge and discoveries to be made in geographical systems that can be translated into delivering solutions for a wide range of societal problems.

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http://www.bartlett.ucl.ac.uk/casa/—Centre for Advanced Spatial Analysis.
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http://www.gisagents.org/—GIS and Agent-based modelling.
http://cs.gmu.edu/~eclab/projects/mason/—MASON Simulation Library.
https://ccl.northwestern.edu/netlogo/—NetLogo, a programmable modelling environment.
https://www.openabm.org/—Open Agent-based modelling Consortium.