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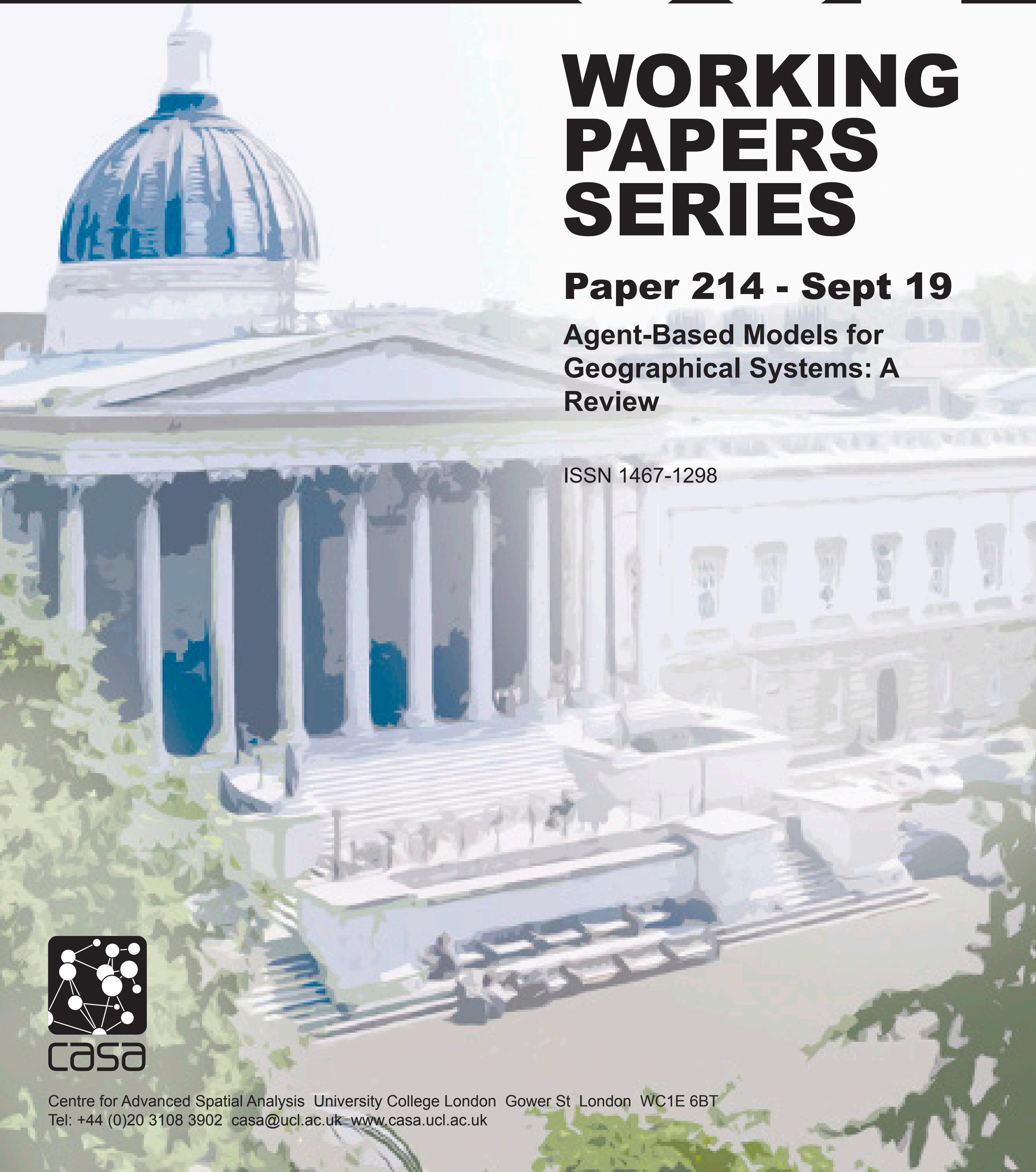

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Agent-Based Models for Geographical Systems: A Review

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Abstract

This paper charts the progress made since agent-based models (ABMs) of geographical systems emerged from more aggregative approaches to spatial modeling in the early 1990s. We first set the context by noting that ABM explicitly represent the spatial system by individual objects, usually people in the social science domain, with behaviors that we simulate here mainly as decisions about location and movement. Key issues pertaining to the way in which temporal dynamics characterize these models are noted and we then pick up the challenges from the review of this field conducted by Crooks, et al. (2008) some 12 years ago which was also published as a CASA working paper[1]. We then define key issues from this past review as pertaining to a series of questions involving: the rationale for modeling; the way in which theory guides models and vice versa; how models can be compared; questions of model replication, experiment, verification and validation; how dynamics are incorporated in models; how agent behaviors can be simulated; how such ABMs are communicated and disseminated; and finally the data challenges that still dominate the field. This takes us to the current challenges emerging from this discussion. Big data, the way it is generated, and its relevance for ABM is explored with some important caveats as to the relevance of such data for these models, the way these models might be integrated with one another and with different genera of models are noted, while new ways of testing such models through ensemble forecasting and data assimilation are described. The notion about how we model human behaviors through agents learning in complex environment is presented and this then suggests that ABM still have enormous promise for effective simulations of how spatial systems evolve and change.

[1] Batty, M., Crooks, A., and Castle, C. (2007) Key Challenges in Agent-Based Modelling for Geo-Spatial Simulation, CASA Working Paper 121: https://www.ucl.ac.uk/bartlett/casa/sites/bartlett/files/migrated-files/paper121_0.pdf

1: From Top Down to Bottom-up

The first spatial models at the geographical scale of cities using digital computers were constructed in the mid-1950s. These models essentially dealt with aggregate populations, largely because the data available had to be aggregated for purposes of confidentiality by the agencies involved in their collection but also because the dominant paradigm widely adopted at the time was based on building models as parsimonious as possible based on Einstein's oft-quoted remark from 1933 that "Everything should be made as simple as possible, but not simpler". Moreover there was a sense that generalizing spatial behaviors was easier if data were aggregated thus implying some deference to the law of large numbers. Modelling temporal dynamics was difficult because of limitations in the availability of data while it appeared that geographical systems could best be modelled as though they were in equilibrium, thus simplifying the quest. Moreover limits on computation were severe and this also reinforced the need to aggregate.

Two models stood out at the beginning. First the Chicago Area Transportation Study (CATS) Commission embarked on an ambitious program of urban model development in 1955 which tied together many aggregate location and flow models that were being fashioned from applications in social physics and urban economics at that time (Carroll, 1956; Boyce and Williams, 2015). Second, from an entirely different perspective, Hagerstrand (1953, 1967) began his work on diffusion that did in fact introduce temporal dynamics and was predicated at the individual level but for purposes of empirical demonstration was made operational at a more aggregate scale. Our purpose for noting these early applications is to reinforce the point that as we have gradually moved towards more disaggregate and dynamic models over the last 50 years – as we moved to agent-based modelling, this was not because we suddenly discovered that modelling individual behaviours over time led to models that worked better and were more relevant to the tasks in hand, but because the constraints on what was possible began to change. Computers, data and spatial software such as GIS (geographic information systems) have improved dramatically over the last 50 years but when this quest began, many researchers did accept that the ultimate goal was to describe geographical systems at as finer grain as possible, both temporally and in terms of human behavior at the individual level, but it was simply not possible at the time.

From these early days however, there remain important insights that continue to dominate agent-based modelling. In particular, the need to ground models in empirical data through validation is still a major priority in that agent-based models generate requirements for much more and very different data from the aggregate equilibrium models of the past. Decision processes that are central to ABMs are hard to observe and many such models rely on plausible hypotheses concerning spatial behaviour that cannot be validated in the traditional way. In this sense, ABMs often conflict with our notions about parsimony, while the emergence of new data at a much greater temporal frequency – big data – although appearing to enable us to grapple with spatial dynamics in a more fundamental way, is often of only superficial relevance. Such data unlike the conventional censuses conducted less frequently, does not yield easily to the kinds of patterns and processes that our ABMs often require.

This then is the context for our exploration of future developments in agent-based modelling for geographical systems at the scale of cities and regions that define human geography. As we have implied, understanding the causes and consequences of individual behavior has been an issue that has taxed geographers for the last 50 years. The development of disaggregate models has always been part of this context but the development of micro-economic theory of the city in the 1960s as typified in 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.*, 2012a). Any changes in the system, or interventions to be modeled were simulated from the top-down i.e. changes were somewhat indiscriminately applied to entire populations, largely because the fine-grain of spatial and temporal location was lacking. This approach resulted in spatial systems being essentially reduced to homogeneous units whereby it was virtually impossible to uncover any new knowledge or insights about emergent phenomena or the micro dynamics of the city (Batty, 2008).

New forms of 'big' data and methods from machine learning are slowly beginning to give added insights into the complexity inherent within geographical systems, and to reveal the importance of individual actions in the evolution of these systems. 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 social and 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 make significant advances 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. This however has yet to be fully demonstrated and there are considerable problems in not only observing relevant data but also in articulating plausible behaviors.

Leveraging this information about individuals and their interactions may however provide researchers with a clearer understanding about the role that complexity plays in shaping spatial 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 progress still required in the "ontological and epistemological representations" of complexity (An, 2012; Grimm *et al.*, 2005; Manson and O'Sullivan, 2006; Parker *et al.*, 2003). Nevertheless, 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. The major group of individual-based methods that has seen a rapid uptake by researchers across the social and geographical sciences in the past 20 years is agent-based modeling (ABM) (Macal, 2016) which advocates the representation and simulation of individuals with their own attributes and behaviors.

By allowing each unique individual to interact, new ideas, information or decision processes emerge. This approach is known as "bottom-up" modeling i.e. changes at the individual level can lead to changes, often referred to as emergence, in macro-level processes. The emphasis within these models on the individual makes it a natural framework to apply within social and geographical systems. Wallentin (2017) lists four reasons, drawn from Dieckmann *et al.* (2000) why individual-based modeling is so popular: mainly because of (i) computer power, (ii) the definition of an easier way to construct models rather than through formal mathematical equations, (iii) the specification of complex system structures that cannot be adequately represented in traditional models, and (iv) the use of observed phenomena that cannot be reproduced satisfactorily using traditional models. 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.

Agent-based models were first proposed in the early 1990s, and while one of the first ABMs to be published in a geographical journal was published in *Geographical Analysis* by Bura et al. (1996) based on simulating the evolution of settlements, ABM is now reaching a point of acceptance as a research tool across the geographical and social sciences (see Polhill *et al.*, 2019 for a discussion). However, there remain significant methodological challenges in areas of recognizing and simulating emergent phenomena, agent representation, construction of behavioral rules, calibration and validation (see Axelrod, 2007; Filatova *et al.*, 2013; Lee *et al.*, 2015; Torrens, 2010). Axelrod (2007) listed a number of challenges facing the modern agent-based modeler which Crooks *et* *al.* (2008) extended. These challenges were presented at a time when ABM was beginning to garner real excitement in the social sciences because of its potential to simulate individual actions. The increase in individual-level data to enrich such models, advances in computing power and software development all presented solutions to some of the original challenges put forward; however while some major questions remain unresolved, advances in data and computing have brought with them a new set of challenges.

This paper reviews the challenges to be addressed in developing and advancing ABM applicable to geographical systems. The first part of the paper will evaluate how well each of these challenges has been met in the decade since the original publication by Crooks *et al.* (2008), before moving in the second part, to critically appraising the new challenges that changes in the research environment, in particular 'big data', has brought about. Finally, we conclude by looking at potential ways to overcome these challenges and provide a road map for future research using GIS in ABM and in the models themselves.

2: Challenges From The Past

2.1: The Rationale for Modeling

In the early days of computer modeling, the first urban models were built to test the impacts of policies rather than to advance scientific understanding *per se* (Batty, 2008).The underlying notion was that, given a good theory, a model could be constructed which would then be validated and, if acceptable, implemented within policy-making (Batty, 1976). This notion has been relaxed over the last two decades, and models are now built to explore all stages of the theory–practice continuum (not just for prediction). This is especially the case for agent-based models, which range from exploratory to the predictive (see Epstein, 2008; Parker *et al.*, 2001). However, a model is only useful for the purposes for which it is constructed, and thus modelers need to be explicit about this and use appropriate verification and validation strategies. For example, if the purpose of the model is for the discovery of new relationships, as illustrated by Filatova *et al.* (2009) in their exploration of the evolution of land markets, the validation strategy might be a theoretical comparison of price gradients. If the purpose of the model, however, is to predict individual movement, as in the case of Crooks *et al*. (2015), one needs to consider quantitative goodness-of-fit measures, for example comparing the output from the individual interactions against aggregated data collected from the real world.

2.2: Theory and Models

One goal of theory is to make the world understandable by finding the right level of abstraction (or simplification; see Miller and Page, 2007). Traditionally in the social sciences, the role of a model has been to translate a theory into a form whereby it could be tested, manipulated and refined. However, with agent-based models (along with computational modeling more generally) models are now often used to develop theory (Axelrod, 2007). That is not to say that agent-based models are theoretically agonistic. There have been several attempts to operationalize existing theories (e.g. Diappi and Bolchi's (2008) attempt at growing Smith's (1979) rent gap theory from the bottom up with respect to gentrification) or to test existing theories (e.g. Pires and Crooks, 2016) or to relax some of the restrictive assumptions of past theories (e.g. adding dynamics and heterogeneous agents to general equilibrium in economic theory; Gintis, 2007). However, a review by Groeneveld *et al*. (2017) found that out of 134 agent-based models of land use they reviewed, only 51 made use of existing theory (the most common being expected utility theory) with respect to agent-based decision-making (which we will return to below). From a more pragmatic point of view, especially from a social sciences perspective, the challenge also relates to which of the many social theories should be tested for it has been noted that for complex systems, such theories might not encompass all important aspects (see Schlüter *et al.*, 2017, for examples). While we do not oppose changing the role of models and theory, the challenge with this shift is that in many agent-based models, the theoretical implications of the model remain implicit and hidden behind many *ad hoc* assumptions which are often poorly articulated.

2.3: Inter-model Comparison

While a growing number of models are being developed for particular applications, these tend to be based on case studies, one-off models or on proofs of concept (Bell *et al.*, 2015; Filatova *et al.*, 2013; O'Sullivan *et al.*, 2016). However there is little in the way of inter-model comparison such as is seen in other areas. Take, for instance, models in the climate science community such as the Community Ice Sheet Model and inter-comparison exercises based on the same initial conditions (e.g. Ice Sheet Model Intercomparison Project; see Nowicki *et al.*, 2016). From an ABM perspective, we are a long way from this. Efforts are being made to compare different models applied to the same phenomena such as the spread of malaria (Ferris *et al.*, 2015), Ebola (Chowell *et al.*, 2017); or common features of models exploring the same phenomena such as growth along frontier regions (Parker *et al.*, 2008b) and slum development (Roy *et al.*, 2014) in order to find out what constitutes the *must-have* features of models exploring similar issues. However, there are no centralized ABM repositories that pool together knowledge, code and data. For this to happen, significant community buy-in would be needed. This in itself is a challenge as agent-based models are being developed across multiple scientific fields and are often developed for specific purposes. Integration of different ABM types and styles is thus an urgent requirement.

Moreover, most modelers do not compare their model to other models (agent-based and other models) that are exploring the same phenomena. Furthermore, unlike in the geospatial realm (e.g. http://www.opengeospatial.org/standards/cdb), there is no standard model or protocol on what constitutes an agent or the decision-making processes that are associated with it. There have been efforts to establish a common framework or protocol for simulation models, often in more specific domains, such as land use, land cover and land markets (Parker *et al.*, 2008a), and socio-ecological systems (Schlüter *et al.*, 2017). However, they serve more as a general guideline for model design and behavioral rules than a protocol that can be easily implemented in the actual model. As a result, although acknowledged by the community, these protocols have not been widely adopted by other modelers so far. It is therefore often left to the model developer and the research question being asked to develop the definition of an agent, which further exacerbates the lack of standard practices in developing agent-based models (a point that is further addressed below). Perhaps the ABM community could take inspiration from the open source R and Python communities where packages are shared and widely used, but this would require modelers to choose specific platforms which also have their drawbacks.

2.4: Replication and Experiment

Replication is one of the main principles of the scientific method. However, this is rarely done or is difficult to achieve in the sciences due to the difficulties in controlling all the variables that pertain to a particular situation (see for example Baker, 2016). We see this also for agent-based models which have multiple parameters, methods and contexts. It is often impossible to outline the entire logic of such a model in a single paper (due to space constraints) but efforts have been made in this area with attempts at designing ontologies and protocols for providing a more detailed model description and aide comparison. These include the ODD (Overview, Design concepts and Details) protocol by Grimm *et al.* (2006), the ODD+D (+Decisions) protocol of Müller *et al.* (2013) and more recently Laatabi *et al*. (2018) extension of ODD+2D (+Decisions and +Data), and the use of UML (Universal Modeling Language) (Bersini, 2012) when documenting key model processes. But the use of such standards is still not the norm for many agent-based modelers. We would also argue that to aide replication and experimentation modelers should consider sharing their models and data. This is because the computational model is the full specification of the theory that the model is built upon and without the codebase (and supporting material), it may be difficult to understand, replicate or experiment with. Thankfully, there are efforts to share and make code and data available such as CoMSES.Net (see https://www.comses.net/).

However, as noted by An *et al*. (2014), code is often only understandable by other modelers and even this can be problematic if it is badly written and poorly documented. It is only through such activities that we can replicate and experiment with agent-based models. Similar efforts with respect to reproducibility of results are also being called on in the geocomputation community more generally (see Brunsdon and Singleton, 2015; Harris *et al.*, 2017).

2.5: Verification and Validation

Verification and validation are challenges for all models that are tested empirically but verification is required if we are to address the challenge of replication and experimentation. To do this, we need to ensure that the formal logic of the computer program behaves as expected, which is an aspect that is often taken for granted. Researchers should document steps taken (e.g. through code walk-throughs and parameter testing) to verify the model.

As we noted at the onset, validation remains one of the biggest challenges (e.g. Batty and Torrens, 2005; Filatova *et al.*, 2013). How can we rigorously evaluate how well the model matches the real-world system it is attempting to simulate? From a geographical perspective, Torrens (2010) notes that this is problematic because the discipline has few techniques for analyzing individual agents in complex systems. The type of statistics and the form of sensitivity analysis that should be used is an issue that has dominated the literature on models of land-use in the land-cover community, for example (Filatova *et al.*, 2013; Pontius *et al.*, 2008). Mandelbrot (1983) argues that good models which generate spatial or physical predictions that can be mapped or visualized must 'look right'. Axelrod (2007) suggests that to understand the output of an agent-based model, it is often necessary to evaluate the details of a specific simulation 'history', and this too is usually a qualitative matter. In contrast, researchers such as Axtell and Epstein (1994) see the validation of models on a scale from qualitative to quantitative, with the highest validation being for a model that attains quantitative agreements with both the emergent macro-structures and an individual agent's micro-behavior.

This challenge sets ABM aside from other traditional forms of modeling. Agent-based models embrace heterogeneous systems that evolve over time, where the linkages between dependent and independent variables are difficult, if not impossible, to observe due to their rich model structure (Batty and Torrens, 2005). Finding appropriately rich and detailed data to validate such systems is difficult and we cannot simply assume that as data gets richer and more widely available from various types of sensors, that agent-based modeling will become any easier.

2.6: Agent Representation, Aggregation and Dynamics

Agents can be represented at a variety of levels (individuals, households, etc.) with their dynamics operating at very different temporal and spatial scales (e.g. from seconds to years). However, little attention has been paid to the selection of these representations or dynamics. Normally modelers choose the agent, representation, dynamics, etc. to meet their research needs. And while it might be easy to assign rules and behaviors to individuals, there is little discussion on how we aggregate these rules and behaviors from the individual level to, say, groups or higher aggregations of agents. With aggregations we lose details, the difficult question being around knowing what details we should lose.

Another issue is how many agents and how many attributes for each agent we should account for. Agent-based modelers often use a sample population, but sampling is not yet a well-developed art in ABM. This representation also raises questions about what are the most appropriate methods for agents to communicate with each other (i.e. via Moore or von Neumann neighborhoods or on social networks). These questions are not new (see, for example, Cioffi-Revilla, 2002) but modelers need to be more explicit with respect to agent representations, why they chose specific spatial and temporal scales, and what data exists to support their assumptions and validate their outcomes.

2.7: Behavior

The role of theory and the representation of agents are both linked to the actions and the behavior that is embedded within agents. There are several approaches that researchers use to incorporate human behavior in agent-based models These range from mathematical or threshold calculations which tend to be the most common for agent-based models (e.g. Epstein and Axtell, 1996) to those that use conceptual cognitive frameworks (e.g. such as PECS framework (Physical conditions, Emotional states, Cognitive capabilities and Social status, Schmidt, 2000; Urban, 2000) which has been used to study crime and conflict (e.g. Malleson *et al.*, 2010; Pires and Crooks, 2017) and 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), and land-use planning (Caillou *et al.*, 2015). These conceptual cognitive frameworks and mathematical approaches for representing behavior can both be considered as rule-based systems and are often applied to tens of millions of agents. The third approach, that involving cognitive architectures (e.g. Soar (Laird, 2012) and ACT-R (Anderson and Lebiere, 1998)) focus on the abstract or theoretical cognition of one agent at a time with a strong emphasis on artificial intelligence compared to the other two approaches and these are not yet capable of extension to the study of large geographical systems..

A criticism that can be leveled here is that modelers do not consider the use of alternative behavioral frameworks or describe in detail why one was chosen over another (see also An, 2012; Balke and Gilbert, 2014; Filatova *et al.*, 2013; Groeneveld *et al.*, 2017; Schlüter *et al.*, 2017). There is a growing call to improve our understanding of cognition in human environmental interactions (Manley and Cheng, 2018; Meyfroidt, 2013) and how best to incorporate human decision-making and behavior in models (e.g. Balke and Gilbert, 2014). Moreover, many researchers have noted that models looking at decision-making do a poor job of describing the decision-making of their agents, and once developed and published are not reused (e.g. Bell *et al.*, 2015; Groeneveld *et al.*, 2017).

This could be related to the fact that human behavior is still not well understood. Most modelers are still developing their own agent-based models in their own disciplinary silos, and there is still very little in the way of standardization or comparison. This is beginning to change with the appearance of frame- works such as ODD + D (Müller *et al.*, 2013) and the Modeling Human Behavior (Schlüter *et al.*, 2017) framework. These frameworks attempt to provide a means for communicating and comparing different theories of individual human decision-making. This echoes other calls to publish more detail on decision models to allow for reuse (e.g. Bell *et al.*, 2015; Groeneveld *et al.*, 2017) through such initiatives as CoMSES.Net. Efforts are being made to develop cognitive frameworks within modeling packages – see for example, the BDI framework in MATSims (Horni *et al.*, 2016) or GAMA (Taillandier *et al.*, 2019) – but this is still rare and not seen in other toolkits/software. The development of standard tools for coding human behavior into cognitive frameworks does not seem unreasonable and would improve the realism within agent-based models.

Another challenge with decision-making is how to enable agents to learn from past experiences, especially those which might impact their future decision-making (Filatova *et al.*, 2013; Groeneveld *et al.*, 2017). Most agent-based models do not explicitly incorporate learning or memory within their decision-making processes (e.g. Benenson and Hatna, 2011; Magliocca *et al.*, 2011). Notable examples include Bennett and Tang's (2006) elk migration model using evolutionary algorithms, Power's (2009) citizen cooperation model, Bone's *et al.'s* (2011) land-use change model which uses reinforcement learning, and Bone and Dragićević's (2010) natural resource extraction model where agents' decision-making evolves over time and is based on past experiences.

However, efforts are needed not only in describing how agents make decisions or in the creation of protocols around sharing models, but also for building good high-fidelity models of human behavior and interaction (Weinberger, 2011). Perhaps data will shed light on this issue, specifically how new sources of data provide new ways to explore how people perceive, use and react to events in the spaces around them. Advances are being made with respect to machine learning and pattern recognition that could add help extract more relevant patterns of human behavior, but we also need to think carefully about how such data can be interpreted in meaningful and intuitive ways.

2.8: Sharing and Dissemination of the Model

The last challenge identified by Crooks *et al.* (2008) involves how we might communicate and share agent-based models with fellow researchers and policy-makers. Traditionally models have been based on the development of intensive and all-pervasive computation, and communicating models was mainly through discussion, simplification and visualization, and through pedagogy in all its various forms (Batty, 1992). Agent-based models can be overtly visual, and through such visualizations one can convey the behavior of the model clearly and quickly over time (Kornhauser *et al.*, 2009). This notion is supported by North and Macal (2007, p. 280) who write that '*visualization is one of the most effective ways to present key model information to decision-makers*'. Two- and three-dimensional visualizations of agent-based and cellular automata models are commonplace, particularly through the animation of spatial model results of land-use change (Clarke *et al.*, 2006; Tobler, 1970) which allows users to see the dynamic recognizable behavior in model results, rather than just exploring models through data and statistics. However, further efforts still need to be made in sharing the underlying modeling processes and activities through frameworks such as the aforementioned ODD and UML diagrams.

However, if we are really to utilize agent-based models in policy decisions we need to directly involve stakeholders in the research. As Gilbert *et al.* (2002) note: 'it is frequently the case that policy-makers dismiss academic research as too theoretical, unrelated to the actual problems they are wrestling with, or in other ways irrelevant to their concerns'. One way of circumnavigating this issue is to explore participatory modeling or companion modeling (Barreteau *et al.*, 2003; Étienne, 2014) which directly involves stakeholders in the modeling processes, including role-playing games to develop and validate model rules, thereby keeping the whole process transparent (Barreteau *et al.*, 2001). While such approaches have been around for over two decades, they have not been widely adopted by the modeling community, but there is increasing evidence of these approaches being used in resource management and urban planning (e.g. Etienne, 2003; Le Page *et al.*, 2015; Semboloni *et al.*, 2004).

Another way of sharing and disseminating models is simply by taking advantage of the internet – not only in disseminating models, but also by allowing users to access, run and explore models in their own browsers. While running agent-based models in real time can be a challenge, especially for complex models which require substantial computational resources, for simple models one can easily use web browsers to disseminate their operation and outcomes. For example, NetLogo provides functionality for models to be run over the web (see https://www. netlogoweb.org/), while Agentscript which is loosely based on NetLogo semantics (http://agentscript.org/) uses JavaScript for simple agent- based models which can be deployed over the web. There have been attempts to share and disseminate models in virtual worlds such as *SecondLife* and video game engines such as *Unreal* and *Crysis* (e.g. Crooks *et al.*, 2011).

2.9: Data Challenges

Agent-based models are all about the individual, and akin to all modeling techniques, large quantities of data are required to create models that can robustly test theories, re-create processes and dynamics and make conditional predictions about the future. Despite the data deluge that we are now experiencing in the wake of the big data movement, there is still a lack of high-quality, linked individual-level data. However, progress is being made here: researchers are increasingly using established approaches such as microsimulation to generate synthetic populations (see Birkin and Wu (2012) for a review) or examine how the demographics of a population impacts agents' behaviors, an area that is referred to as agent-based computational demography (see Billari and Fürnkranz-Prskawetz, 2003). This is an important next step, but work is also needed to connect these synthetic populations to realistic social networks (Burger *et al.*, 2017; Wise, 2014), grounded in observed data (such as average group sizes, number of connections) which can be gained from anthropological and psychological studies (e.g. Dunbar and Spoors, 1995), or from new sources of data (e.g. social media, mobile phones). These enable us to understand the connections and ties between people or to test whether or not findings from previous studies in the social sciences are applicable to larger case studies. For example, Dunbar (1998) proposed that humans can maintain around 150 stable face-to-face relationships based on his own observations and the advent of new data means that we have the opportunity to test this observation at scale. Researchers have begun to do this; for example, Dunbar *et al.* (2015) found that online social networks (e.g. Facebook) had similar structures to offline face-to-face networks, while MacCarron *et al.* (2016) found similar trends with mobile phone data.

Using spatial data for building the artificial worlds in which our agents operate is quite straightforward. However, if we are to reuse models or to build new ones, improved methods are needed for reading data into models for model initialization. Within the literature, there is little discussion about the difficulties with and time-consuming nature of preparing data for input into the models (data cleaning, formatting, etc.), limiting such models with respect to rapid prototyping. In addition, there are multiple types of data involved. Many geographically explicit models use both raster and vector data and in some instances will also require networked data (i.e. social connections) in the form of graphs. Furthermore, many applications note that one of the major limitations of their models is lack of fine-scale behavioral (and movement) data sets (e.g. Batty *et al.*, 2003; Torrens, 2014). For example, it is extremely difficult to get data about slum locations (Mahabir *et al.*, 2018), population information and social connections between inhabitants of a city, along with the current 'mood' of the population. Advances with open source libraries like the Python packages of Shapely (https://pypi.python.org/pypi/Shapely) and Geopandas (http://geopandas.org/) make manipulating data and formatting it for use with models easier, but there is still a significant amount of time needed to prepare data for initializing a model for a new area. Scripting such procedures would also help make them applicable to new areas along with the use of standard data formats (e.g. ESRI shapefiles) but in general, newcomers to the field of agent-based modeling struggle to get data into models, given limited hands-on training or the lack of available tutorials (Taillandier *et al.*, 2019).

3: Looking Ahead

In this section, we will now turn to the opportunities that lie ahead for agent-based modeling and geographical systems, especially as computing power, storage capacity and data volumes and type increase. As Torrens (2010) notes, ABM promotes spatial thinking in the sciences where such models have been fused with GIS to study a diverse range applications, including agriculture (e.g. Deadman *et al.*, 2004), avalanches (e.g. Kronholm and Birkeland, 2005), criminology (e.g. Malleson *et al.*, 2010), epidemiology (e.g. Shook and Wang, 2015), economics (e.g. Bert *et al.*, 2015), geomorphology (e.g. Favis-Mortlock, 2013), gentrification (O'Sullivan, 2001), housing markets (e.g. Torrens and Nara, 2007), invasive species (Anderson and Dragićević, 2018), natural hazards (e.g. Dawson *et al.*, 2011), urban growth (e.g. Xie *et al.*, 2007; Xie and Fan, 2014), urban shrinkage (e.g. Haase *et al.*, 2010), the rise of cities and regions (e.g. Pumain, 2012), slums (e.g. Augustijn-Beckers *et al.*, 2011) and traffic models (e.g. Horni *et al.*, 2016). The list is long and detailed and is by no means complete but it serves to show how ABM has many diverse applications to geographical systems. By utilizing GIS, we can initialize agent-based models to real-world locations and provide spatial methods for relating these objects (agents) based on their proximity, intersection, adjacency or visibility to each other.

3.1: Big Data and Agent-Based Modeling

The majority of published applications use more 'traditional' data types. This partly due to the fact that modelers are more comfortable manipulating traditional sources of data (e.g. census data; see Robinson *et al.*, 2007) than mining new forms of data, but it is also due to the limits posed by new sources of data that are often unstructured and thus unsuited for ABM or are too noisy, biased or inaccurate. Nevertheless it is clear that the rise of big data represents a significant opportunity for agent-based modeling. New forms of data provide us with new avenues through which to explore how people perceive, use and react to events in the spaces around them, and there is some potential to incorporate these observations into our models in near real time. Moreover, many of these sources of data allow us to examine the connections between people, organizations and space, thus offering a new perspective with which to construct artificial worlds, build environmental layers and derive behaviors that motivate agents to make certain choices and take certain actions. It is clear that big data is making, and will continue to make, a considerable impact on future agent-based modeling but as yet, the application of ABM does not make a strong distinction between different types of temporal detail and thus a whole range of applications to the near real-time city beckons.

By building agent-based models with information obtained from big data, we can simulate society across many application areas in terms of who the agents are, where they are located (or where the study area is), what they are doing or what they are responding to, and why this might be the case. For example, there is a growing amount of work on exploring how crowdsourced data can be utilized to aid humanitarian relief efforts after natural disasters or disease outbreaks including the Humanitarian OpenStreetMap Team and Ushahidi (see Hu *et al.*, 2017; Meier, 2015, for more information). One of the most notable and early examples was after the 2010 magnitude 7 earthquake in Haiti that killed 230,000 people and left 1.6 million people homeless. Volunteers mapped the devastation and provided a near real-time map of the current situation on the ground. Crooks and Wise (2013) utilized such information as the foundation for their agent-based model of post- disaster relief operations over a span of a week. Specifically, they explored the placement of relief centers and how the affected population might get to the aid centers based on the level of devastation seen on the ground, and agents utilized the road network for navigation which was sourced from OpenStreetMap. Spatial data can act as a basis for the artificial world (a base map, so to speak) that agents can inhabit. Crowdsourced data gives a unique insight into refugee camps allowing the exploration of diseases spreading or the outbreaks of riots to be examined at a detailed spatial scale (see Crooks and Hailegiorgis, 2014; Pires and Crooks, 2017).

Other researchers, such as Malleson and Birkin (2012) and Lovelace *et al*. (2016) have started using social media to explore how people move through space. From mining such data they were able to derive information to classify individual behaviors and begin to develop models of that explored behavior through space and time that can ultimately be used to model travel-to-work patterns or similar activities.

Building on such movement analysis from social media and OpenStreetMap to build artificial worlds, Wise (2014) created synthetic populations of agents and mined social media to define people's moods (sentiment) during a wildfire event and subsequent evacuation in Waldo Canyon, Colorado Springs, in 2012. Using tweets harvested during the event, Wise (2014) first manually classified a number of tweets as of positive, negative, or neutral sentiment with respect to the wildfire. Once this training data set was created the remainder of the tweets were analyzed to derive the sentiment of all the remaining tweets during the event using the AFINN lexicon (dictionary)

(Nielsen, 2011). The results of this demonstrated where the peak of Twitter activity corresponded to the peak of the wildfire. This social media data set was directly used to inform agent-based decision-making. For example, if one of the agents (i.e. a Colorado Springs resident) knew that the fire was nearby, this information was passed along their social network to other agents who then decided whether to evacuate or not. The movement (evacuation) patterns were then validated using congestion data that was again harvested from the crowd (in this case images and news reports).

The examples above offer a snapshot of the potential of using big data for building agent-based models focusing on *who* (the agents were), *where* (agents located in space and time), *what* (the phenomena was being modeled) and *why* (agents make decisions the way they do). However, these applications focus on relatively short time frames (from hours to weeks), while traditionally models of the low frequency/fidelity geographical systems have tended to focus on years and decades. Here agents are constantly interacting with each other and their environment at finer spatial and temporal scales than more traditional models. It is in this sense that agent-based modeling is focusing on understanding the bottom-up mechanisms that make use of the physical and social infrastructure to drive the complex systems. To some extent big data, especially that coming from social media, is also generated through a bottom-up approach and offers a valuable means of exploring cities. The data is dynamic, immediate, and relates to how people interact in space and time.

3.2: Model Integration

While there has been a proliferation of agent-based models, many of these tend to look at only one aspect of a geographical system. Such models can range from the small-scale movement of pedestrians to the spread of diseases or the growth of slums. One reason for this piecemeal approach at looking at geographical systems is limited computational power and the availability of fine-scale data on which to base individual behaviors. This is now changing. In the past geographically explicit models were limited to small numbers of agents (due to computational and data constraints), but with the growth in computational power and data availability one can simulate millions or more of agents. But if we are to address larger societal issues (e.g. climate change, urban change), these individual models will need to be integrated as each just reflects at one part of the bigger geographical puzzle.

However, to date there are no geographically explicit agent-based models that simulate a city in its entirety. The challenge is that many models focus on just one aspect (or subsystem) of city life (e.g. travel to work, residential location, the spread of disease, the economy) and treat other urban processes or subsystems as exogenous variables, ignoring the fact that all processes within cities are intricately linked. For example, transportation impacts residential locational decisions or how one navigates around cities. While this piecemeal approach to examining cities is useful, to truly understand cities we need to view them as 'systems of systems'. Returning to the notion of complexity, we can view cities as hierarchical and composed of interrelated subsystems (parts within parts) in which each subsystem is interdependent but connected to many other subsystems. Such subsystems may plausibly be thought of as self-organizing. In economics, for example, national and global markets evolve from locally interacting agents all pursuing their own goals. At a city level, one could consider town centers or sub-centers as system structures. If we look at the connections between these elements we have a hierarchy, echoing ideas about systems that are near-decomposability (Simon, 1969; 1996): here a system (the city) has subsystem components interacting among themselves 'in clusters or subgraphs, and interactions among subsystems being relatively weaker or fewer but not negligible' (Cioffi-Revilla, 2017). But it is not just the town centers and other elements that are connected but also urban processes and this mirrors the sort of complexity that pertains to city systems, thus making comprehensive ABMs for cities in their entirety hard to articulate and construct

This systems approach to understanding cities is not new and goes back to the first urban models (Batty, 2013). For example Christaller's (1933) central place theory noted the hierarchical structures of villages, towns and cities. Simon (1969; 1996) argues that hierarchy is a fundamental property of how a complex system holds itself together, while Batty (2013) notes that "hierarchical organization from the bottom-up is essential for evolving systems and that hierarchical structures are the way nature and society develop robust and resilient structures" (Batty, 2013). However, these subsystems do not operate in isolation. In the short term, they might appear to be independent of the rest of the larger system, but in the long run they are indeed dependent on the aggregate system behavior. As Lippe *et al.* (2019), writes, "T(t)here is a need for ABM to cross the gap between micro-scale actors and larger-scale environmental, infrastructural and political systems in a way that allows realistic spatial and temporal phenomena to emerge". For example, most traffic models just explore traffic, while residential location models do not take into account the impact of traffic congestion on residential decisions (Wise *et al.*, 2017).

To model a city or selected subsystems, we need to combine/integrate smaller models. Perhaps the best approach is through model integration and coupling. The coupling of various models has been common in more traditional modeling domains, especially in land-use–transport interaction (LUTI) models whose purpose tends to be to test new transportation schemes and/or new land-use developments and their impacts. One example of an extended LUTI model is the integrated assessment model by Walsh *et al.* (2011) designed to explore urban sustainability in the context of climate change. This framework couples various models together (e.g. a regional economic input-output model, an employment, population and land-use model, a GIS model, and a flood model) to explore climate impacts, adaptation options and greenhouse gas emissions. Such coupling of agent-based models with others is still in its infancy but is being discussed (e.g. Kettler and Lautenschlager, 2017; Taylor *et al.*, 2004), and we would expect this hybrid form of modeling to continue in the future, mixing and matching the best from many different simulation frameworks which reflect different styles of model.

The integration of different modeling styles (e.g. microsimulation, system dynamics) as opposed to straightforward coupling, should be considered as the choice of modeling approach depends on the purpose and needs of the research (Martinez-Moyano and Macal, 2016). For example, agent-based models are good for modeling problems that lack central coordination (Macy and Willer, 2002) and where emergence is key. If emergence is not central to the problem, other approaches might be more suitable, for example, loosely coupling agent-based models of evacuation with flood-risk models to understand and predict the impact of such an event (e.g. Dawson *et al.*, 2011; Wang *et al.*, 2016), or combining a computational fluid dynamics model of a contaminant plume and an agent-based model of movement to explore evacuation design and exposure risks (Epstein *et al.*, 2011). MATSims has been linked to a discrete choice model of residential location (Ziemke *et al.*, 2016), while Park *et al.* (2017) coupled an agent-based infection model to the Global Change Assessment Model to explore corn production. North *et al.* (2015) combined a system dynamics energy security model with an agent-based conflict model to explore how changes in oil prices could impact a fragile nation. Finally, Bert et al. (2015) integrated a land rental market with an agent-based agricultural model to explore land-use change in Argentina.

Note that we are not the first to consider this issue (see, for example, Heppenstall *et al.*, 2012b). O'Sullivan *et al.* (2016) also notes that agent-based models should be integrated as many models can capture complicated patterns and processes, or different modeling styles should at least be compared in the same research domain. However, if we are to merge models, we need to consider what are the appropriate spatial (e.g. centimeters, meters, kilometers) and temporal scales (e.g. seconds, hours, years) and behavioral processes associated with the actors in each of these subsystems. This poses a significant challenge with respect to capturing behavioral processes over such diverse spatial and temporal ranges. Any urban model or model component must account for these dynamic characteristics in time, space and behavior. We should also be cautious with model integration; the first generation of urban models attempted to capture too many details in some of their parts and too few in others and were criticized for being too complicated and data-intensive, ironically at a time when data and computational power were highly limited (Lee, 1973).

One major stumbling block with model integration is that, despite advances in computing power, the integration of numerous large, complicated models will continue to be extremely difficult to run in reasonable amounts of computer time. There are methods for scaling agent-based models such as distributed computing (e.g. DMASON; Cordasco *et al.*, 2013) using cloud based servers or using high-performance computing (e.g. Repast HPC; Collier and North, 2013), but these are still very much under development. There are a growing number of companies specializing in scaling agent-based models such as Improbable's (https://improbable.io/) SpatialOS or Sandtable's Sandpipr cloud platform (https://www.sandtable.com/) which have the potential to offer solutions to these problems but it is early days yet and our experience with such cloud-based computing and ABM is limited.

For model integration to become a standard part of the agent-based modeling community, more formal protocols are required for model communication. Some progress is being made in this area; for example, NetLogo has an extension called LevelSpace (Hjorth *et al.*, 2015) which allows one to run an arbitrary number of concurrent NetLogo models simultaneously which can communicate with each other. For example, a model of human population growth could be tied to a model of food production which in turn could be linked to a climate model. Each one of these models can potentially influence each other; for example, as the population grows there is more demand for food, and the crop model might need a certain temperature or amount of rainfall, which could be input from the weather model.

We also see linking various subsystems as a rich vein of future work. The future of this area will be characterized by big data powering complex agent-based models for large-scale simulations. Moreover, it is only through model integration that we might be able to provide potential solutions for the series of grand societal challenges such as urban growth, climate change, security and sustainability, aging, migration and the diversity of health issues that now dominate contemporary society.

3.3: Uncertainty and Ensembles

As the agent-based modeling method matures, there are opportunities to begin to adapt useful methods from longer-established fields in order to improve its rigor. One example of this is with respect to how agent-based models deal with *uncertainty*. Uncertainty can arise in models through noise in the input data that are used to parameterize the model or because the model rules themselves are poorly specified (i.e. the model does not adequately represent the target system). Other fields, particularly the environmental sciences such as meteorology and hydrology, have decades of experience in developing methods to quantify and manage uncertainty.

One of these is *ensemble modeling*. An 'ensemble' is a group of models that are run simultaneously. As the models are probabilistic, they naturally diverge during the course of a simulation. By analyzing the range of model results across an ensemble of models, it is possible to begin to better understand how uncertain the outputs are. For example, if most models are broadly in agreement with respect to a particular result, then it is possible to be reasonably certain that that result is a likely outcome. In the cases where the models in the ensemble are in disagreement about a result, then there is more uncertainty. This has serious implications for any conclusions that are drawn from the results and so more rigorous treatment of uncertainty has the potential to improve the trust that others (including policy-makers) can have in the results of an agent-based model. By presenting results from models alongside their uncertainty, modelers have an opportunity to more rigorously represent the reliability of their predictions. People are generally appreciative of the uncertainty associated with, for example, weather forecasts ('there is a 40% chance of rain today') so should be comfortable with the uncertainty generated by an ensemble of agent-based models.

3.4: Data Assimilation

Another useful innovation from the physical sciences that agent-based models could adapt is data assimilation. As already discussed, models of complex systems often diverge rapidly from some initial starting conditions. One way to prevent this would be to occasionally incorporate up-to-date data and adjust the state of the model accordingly. 'Data assimilation' refers to a suit of techniques that allow new observations from the real world to be incorporated into models (Lewis *et al.*, 2006). Many of the most commonly used data assimilation techniques use large numbers of simultaneous models so there is a large overlap with ensemble modeling.

Although there are similarities, data assimilation is quite different to typical agent-based parameter estimation (and also calibration). Parameter optimization does not consider the state of the model during runtime. To determine optimal parameter values, algorithms assess the fitness of a model (i.e. how similar it is to some real data) once a simulation has finished. Even when optimal model parameters have been found, there is usually a degree of uncertainty in the model (agent decisions are usually probabilistic) so divergence will still be a problem. Rather than finding optimal parameter values (although they can do this as well) data assimilation techniques adapt the state of the model itself to try to bring it towards observational data. The techniques themselves have largely evolved in fields such as meteorology (i.e. to incorporate up-to-date environmental data into weather forecasts), and it is not clear whether they are appropriate for use in agent-based modeling. Some have begun to explore this area (Wang and Hu, 2015; Ward *et al.*, 2016) but only with the simplest agent-based models. The marriage of data assimilation methods and agent-based models could be transformative for the ways that some systems (e.g. 'smart' cities) are modeled.

3.5: Learning Agents

Despite advances in our field, many of the models we create to represent human behavior are simplistic at their core. It is common to see assumptions of optimality, be it cost, time, or distance, and omniscience at the heart of simulation, and intrinsic within this is the assertion that this provides an adequate representation of human behavior and knowledge. Yet both intuitively and academically we know this not to be true – years of research in psychology and geography have identified a range of biases and limitations in human abilities that inevitably lie at the heart of the systems we seek to replicate (Gigerenzer and Selten, 2002; Simon, 1972).

Modelers are not without methods to describe these behaviors. Various behavioral models and frameworks address some of these components, and new forms of data provide quantitative insights into the nature of these behaviors. Yet limitations pertain in terms of data requirements and technical expertise, and the imposition of the modeling structure naturally leads to a simplification of behavioral complexity, rather than an exploitation of the full depth contained within our observations. Many of these methods are criticized for a lack of behavioral realism (Balke and Gilbert, 2014) or require significant learning curves to allow their proper use.

One approach that could hold promise in improving the description of human behavior and population-level heterogeneity is reinforcement learning (RL). Unlike other behavioral modeling methods, where agents are given the behavioral model to complete a task, RL agents attempt to complete a task in an efficient way, given a set of observations. The design of the environment, observations and task reward are set by the modeler, but the behaviors required to achieve that goal are not (Sutton and Barto, 2018). In doing so, the modeler gives up some control on design, but provides an environment within which the artificial agents can learn to replicate human actions. There are a variety of learning approaches within RL, but some are underpinned by psychological and neurological theory (Dayan and Daw, 2008; Gershman and Daw, 2017), yielding us a robust framework for building agent behavioral models. To this point, there has been minimal crossover between developments in RL and their implementation in geographic agent-based modeling (Bone and Dragicevic, 2010; Bone *et al.*, 2011) with a primary focus being placed on optimizing agents for adaptive control (Balaji *et al.*, 2010; Tumer and Agogino, 2007).

A particularly relevant area for improved learning models within ABM lies in spatial learning. We know from a range of studies from diverse academic disciplines that the way humans recall, describe, and navigate through geographic space is non-trivial (Gärling and Golledge, 1989; Montello, 1998). Through studies in behavioral geography, psychology and neuroscience (Golledge, 1999), we have a reasonable understanding that humans remember and recall spaces with bias, error and skew, and are bounded in their ability to navigate through space by their prior experiences. The reasons for these limitations are due to the way our brains have evolved, with specific brain cells that suggest an evolved spatial learning process based on landmarks (place cells), direction (head direction cells), regions (border cells), and spatial association (grid cells) (Moser *et al.*, 2008).

Despite these findings, our modeling of human behavior in space tends to assume that agents have 'perfect' spatial knowledge and are able to optimize their choices in moving around it. Furthermore, in building on GIS data, models build in an implicit Euclidean representation, which translates into the way agents are modeled to make decisions. Only a handful of simulation models have sought to integrate aspects of spatial cognition and bounded learning (Manley and Cheng, 2018; Manley *et al.*, 2015).

Within the spatial context, a promising route forward could be allowing the agents to learn their 3D environment for themselves. Through methods such as deep reinforcement learning, where positive behaviors are 'learned' through a repeated exposure to an environment, deep neural networks, which capture uncertainty and incomplete knowledge representations, and large-scale individual tracking data, it may be possible to teach agents how to navigate spaces as if they were human. These 'spatial learning' agents may both better reflect the actual behaviors of humans, and model their behavior under changing conditions. Progress is rapidly being made that replicate cognitive processes of agent behavior (Banino *et al.*, 2018), social interactions (Leibo *et al.*, 2017), and autonomous vehicle interaction with 3D spaces (Shah *et al.*, 2018), but integration into geographical modeling remains both a challenge and an opportunity.

4: Conclusions

Understanding the complexity of the geographical systems around us is a fundamentally important challenge. Through a deeper grasp of how our world works, and an improved ability to predict future changes, we can seek to make improvements or militate against threats. ABM is a highly promising methodology for tackling geographical complexity, offering us a framework for analyzing the deep systemic interactions that take place within and between socio-technical actors and the wider environment. And yet, in this statement we reveal the ongoing limitations of the methodology. ABM remains a relatively immature discipline, and during our discussion we have revealed a vast variety of approaches, languages, theories and methods all in wide use. As such, our verdict of 'highly promising' reflects the immaturity of the field, and the need to do much more to fully achieve its potential.

This does not imply a negative outlook for ABM. It is a highly active and diverse field, enjoying wide success in a variety of contexts. The increasing availability of data, growing computational resources, deeper multidisciplinary thinking, and the simple intuition of the approach all mark ABM as an approach with a rosy future (see Waldrop, 2018). Nevertheless, to achieve full maturity and credibility, ABM for geographical applications requires focus in a number of areas.

Perhaps the most pressing need is for a deeper focus on scientific method – specifically, replication, validation and progression. As highlighted above, despite the variety of ABM work being carried out, the field lacks a cohesive direction of progress. New (hopefully excellent) ideas are implemented into new (hopefully excellent) models, but fail to properly integrate the beneficial work that has gone before. New models do not necessarily need to extend previous modeling work, but some alignment with respect to theory, spatial behavior, or development methodology would enable improved interpretation and recognition of progress. This will not occur in the dark, and modelers must be open with their creations, sharing methods and code openly, allowing and assisting others to investigate and build on what they have done. Replication of results should be encouraged, and integrated as an important element of model development. While the availability of new data means researchers will be drawn to new ideas and approaches, control over how these models are integrated into a wider understanding is needed. This means that we need to continually revisit how these models can be used to make conditional prediction in the wider context of policy and planning.

Agent-based modelers should also be braver about presenting this approach as an alternative to other methodologies. Often the intuitive simplicity and methodological diversity of the approach means it is seen less favorably than more mathematical approaches based on statistical analysis, particularly in this age of data science. But ABM enables one to capture a greater diversity of behavior than most other methods, and lends itself very suitably to integration with new forms of data. However, modelers must be disciplined in how they verify and validate their models, adhering to the now well-established set of methods for testing a model.

Agent-based modelers must also talk with those from other modeling disciplines, and be open about the strengths and weaknesses of the approach and routes towards achieving progress. We should also engage more deeply with the public and with policy-makers, and isolate and develop examples of where ABM is contributing positively to public life (beyond the conventional examples of pedestrian modeling and movie special effects). There is an exciting future ahead for this style of modeling., but the future development of such agent-based models must thoughtfully deliver the promises that it currently offers.

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