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Review

Challenges, tasks, and opportunities in modeling agent-based complex systems

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ABSTRACT

Humanity is facing many grand challenges at unprecedented rates, nearly everywhere, and at all levels. Yet virtually all these challenges can be traced back to the decision and behavior of autonomous agents that constitute the complex systems under such challenges. Agent-based modeling has been developed and employed to address such challenges for a few decades with great achievements and caveats. This article reviews the advances of ABM in social, ecological, and socio-ecological systems, compare ABM with other traditional, equation-based models, provide guidelines for ABM novice, modelers, and reviewers, and point out the challenges and impending tasks that need to be addressed for the ABM community. We further point out great opportunities arising from new forms of data, data science and artificial intelligence, showing that agent behavioral rules can be derived through data mining and machine learning. Towards the end, we call for a new science of Agent-based Complex Systems (ACS) that can pave an effective way to tackle the grand challenges.

1. Agent-based complex systems

Agent-based complex systems (ACS), largely equivalent to complex adaptive systems, often include heterogeneous subsystems, autonomous entities, nonlinear relationships, and multiple interactions among them (Arthur, 1999; Axelrod and Cohen, 1999; Crawford et al., 2005; Levin et al., 2013). Individual actors make decisions and interact with one another or with their local and/or remote environment, giving rise to or shaping emergent outcomes which in turn affect the agents' behaviors and interactions (Coleman, 1987; Railsback and Grimm, 2012). Such systems may bear complexity features such as path-dependence, contingency, self-organization, and emergence not analytically tractable from system components and their attributes alone (Bankes, 2002; Manson, 2001; National Research Council, 2014).

A large amount of efforts have been invested in exploring complex systems (Axelrod and Cohen, 1999; Grimm et al., 2005; Helbing et al., 2015; Levin et al., 2013, 2012; Manson, 2001) and the corresponding methods and tools (Cardinot et al., 2019; Kravari and Bassiliades, 2015; Railsback et al., 2006) from scientists of various backgrounds. In biology, cell simulation has included thousands of genes and millions of molecules (Karr et al., 2012). In chemistry, complex molecules have been investigated digitally in terms of their structure and properties

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before they are manufactured in the lab (Lewars, 2011). In climate science, the whole Earth models couple atmospheric and ocean circulation dynamics to study global warming at ever-finer spatiotemporal resolution (Lau and Ploshay, 2013). Particularly worth of mention is the contribution from physics, which—traditionally using the language of mathematics—focuses on theory and empirics (e.g., experiment results). Later on, physicists started to define and leverage complex systems theory as they were engaged in explaining deterministic chaos, quantum entanglement, protein folding, spin glasses, etc. The system behavior crucially depends on its details such as interactions between constituent parts, which lead to collective behavior and define the macro-state (Perc, 2017). The macro-state would in turn affect the states of constituents and interactions, making them co-evolve over time. All such observations and explorations, especially those in statistical physics and quantum mechanics, have substantially nurtured the growth of complex systems theory. For detail on the contribution of physics in complexity science, we refer to a review article (Holovatch et al., 2017). Also studies of complex adaptive systems have benefited from—and are instrumental to—efforts in understanding global macroeconomic network, stock market, political parties, social insect colonies, immune system, and internet connections (An et al., 2020; Axelrod and Cohen, 1999; Cumming, 2008).

In this context, more progress on ACS theory development is needed in social, ecological (Grimm and Berger, 2016), and social-ecological sciences (An et al., 2020, 2014a), Taking social-ecological (or human-environment) research as an example: ACS models are lagging behind in this field and have in particular not yet developed a productive culture of model analysis and testing (Schulze et al., 2017). In social and ecological systems, more efforts and achievements have been obtained (see Sections 3.1 and 3.2), yet they are fragmented, less communicated to other disciplines, and/or not distilled into complex systems science level. The development of a culture of system representation and exploration (including model analysis and testing) may enable scientists to develop ACS models and principles, distill commonalities from locale-specifics, test and generalize site-independent hypotheses, and ultimately formalize theories applicable to the ACS under investigation. This context leads to our efforts in this synthesis paper regarding modeling ACS.

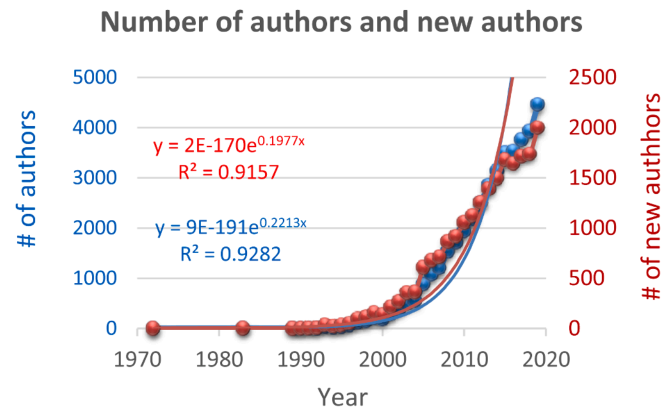

Fig. 1. Number of authors and new authors over time (data as of 17 February 2020). Blue and red represent authors and new authors who develop and use ABM over time, respectively. For data collection see An et al., 2021).

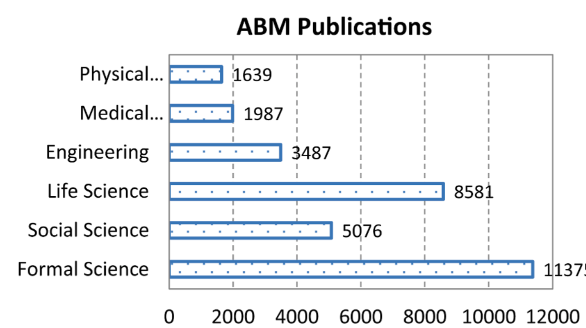

Fig. 2. ABM publications by scientific branch (data as of 17 February 2020. For data collection see An et al., 2021). The term "formal science" represents disciplines concerned with formal systems, such as logic, mathematics, statistics, theoretical computer science, information theory, game theory, systems theory, decision theory, and portions of linguistics (http://en.wikipedia.org/wiki/Formal_science; last accessed February 12, 2021).

2. History of agent-based modeling

Agent based models (ABMs; for agent-based modeling we use the acronym ABM throughout the paper) adopt a realist, typically objectivist, ontology, where observable actions are modeled with a detailed representation of agents that live in complex environments (Grimm and Railsback, 2005; Stillman et al., 2015). In ecology, ABMs are often called individual-based models. The ABM approach focuses on the uniqueness of individuals and interactions among them or between these individuals and the associated environment(s). ABMs are used whenever one or more of the following aspects of real ACS is considered essential for answering a certain question:

- agents are different in some variables and such differences are essential for agent behavior and/or systems dynamics;
- agents interact locally (in space or networks);
- agents live in time-varying and heterogeneous environment(s);
- agents adapt their behavior to the current (and sometimes projected future) state of themselves and their environment in their pursuit of a certain objective.

These aspects, particularly agents' flexible and diverse behavioral responses observed in human society or nature, are not easily found in simplified models (Evans et al., 2013). Hence ABM allows for studying a wider range of behavioral phenomena or processes and addressing many empirical and theoretical problems (Arthur, 1999; Axelrod and Cohen, 1999; Lindkvist and Norberg, 2014; Manson, 2001), which are axiomatically complex. Technologically, agent-based modeling has emerged and prospered with the advent of increasingly available computing power, new forms of data, and capability of data handling and storage. Given complexities in ACS, it has been suggested that the ABM approach be employed to understand, harness, and improve (rather than fully control) ACS' structure and function, taking innovative actions to steer the system of interest in beneficial directions (Axelrod and Cohen, 1999).

The use of agent-based models for empirical study and scientific inquiry has increased rapidly among various scientific communities over the last two decades. The number of authors and new authors who develop or use ABMs has been steadily increasing at an exponential rate since the mid-1990s (Fig. 1), spanning research fields including ecology, epidemiology, land system science, sociology, and archaeology (Fig. 2; see also the paper by Vincent, 2018). Further advances in ABM have led to the founding of the Journal of Artificial Societies and Social Simulation in 1998 and several scientific associations in both Europe and the US in the 2000s. As a climax of ABM popularity, a PNAS special issue was published in 2002 as an aftermath of the National Academy of Sciences Sackler Colloquium, where ABMs were greeted with enthusiasm because of the potential "revolution" it may bring up in scientific inquiry (Bankes, 2002).

This hype faded with time as "scientists sometimes tend to rush to a new approach that promises to solve previously intractable problems, and then revert to familiar techniques as the unanticipated difficulties of the new approach are uncovered" (Grimm and Railsback, 2005, p. xi).

Progress in agent-based modeling has been slower than initially anticipated (Bonabeau, 2002; Huston et al., 1988) in critical areas such as ABM validation and identifying outcomes that differ from or are better than those from other types of models (An et al., 2014a; Grimm et al., 2005; Grimm and Berger, 2016; Grimm and Railsback, 2005; Rindfuss et al., 2008; Thiele and Grimm, 2015). Interestingly, such questions are not always asked of other model types. Subsequent progress with advancing ABM methodology has been slow, reflecting the fact that any tool for tackling complex systems comprised of agents in different contexts has to cope with complexity inherent in such systems. These challenges can explain—at least partially—frustration with the approach and even general doubts about its usefulness (e.g., Couclelis, 2002; Roughgarden, 2012).

With the recent appearance of new forms of data (e.g., micro-level or individual-level data from different sources such as citizen sensors, smart meters, and remote sensing) and the unprecedented ability to better understand the system(s) under investigation, the popularity of ABMs as a modeling tool continues increasing (Fig. 1). ABMs are useful for integrating a variety of data and models from multiple disciplines, for addressing problems across spatial, temporal, and organizational scales, and for various mind experiments, hypothesis testing, or scenario explorations (An et al., 2014a, 2005; Borrill and Tesfatsion, 2011, 2011; Gimblett, 2002; Grimm, 1999). ABMs are also increasingly being used to facilitate cooperation in inter– or transdisciplinary settings where they support communication and understanding across disciplines and knowledge systems of scientists and non-scientists, for example via participatory modeling (Ramanath and Gilbert, 2004; Voinov and Bousquet, 2010).

3. ABMs in ecological, social, and social-ecological systems

3.1. ABM in ecological systems

In ecology, the use of ABMs (often referred to as individual-based models or IBMs) started about 10 years earlier than in other disciplines (DeAngelis and Gross, 1992; Huston et al., 1988; Liu, 1993). Initially ABMs were used to take into account heterogenous individuals and interactions between them at the local, not global, scale. Increasingly, ecological ABMs are also representing adaptive behavior. In ecological ABMs, organisms are simulated as agents that move, fight or flee, browse or feed, reproduce, or form and maintain territories based on some internal state of each organism and its (often imperfect) knowledge of the environment with some goals such as optimal fitness (DeAngelis and Diaz, 2019). In an increasing proportion of these models, individual organisms make "decisions" to achieve some goal that increases fitness, such as growth or survival. These models have focused on the importance of many individual-level behavioral differences such as "bold" vs. "conservative" behavior in fish, various responses to intra-and inter-specific competition, and tradeoffs between growth, mortality, and early and late reproduction. All such differences affect community dynamics, making ABM highly useful to account for details in individual behavioral traits in addition to age, sex, body mass, and so on as well as feedback effects (DeAngelis and Diaz, 2019).

Ecologists contributed to the maturation of agent-based modeling through developing a standard format for model formulation and communication named the Overview, Design concepts, Details (ODD) protocol (Grimm et al., 2006; Polhill, 2010; Polhill et al., 2008). Other contributions from ecologists include testing a general strategy for achieving structural realism via verification and validation (e.g., through "pattern-oriented modelling" (Grimm et al., 2005; Grimm and Railsback, 2012a), the increasing use of "first principles" (e.g., energy budgets, physiology, objective seeking, heuristic decision algorithms) to represent agents' behaviors (Martin et al., 2013; Railsback and Harvey, 2013, 2002; Scheiter et al., 2013), and the establishment of sensitivity analysis as a required element of model analysis (Ligmann-Zielinska et al., 2020). Furthermore, ecologists have developed a general framework for designing and documenting model evaluation, which is particularly important for models developed for decision or policy support (Augusiak et al., 2014; Grimm et al., 2020a, 2014; Schmolke et al., 2010).

Ecology is also pioneering the modeling of adaptive decision making. There are situations that traditional models—mostly those aiming to optimize certain long-term goals—cannot handle well. For instance, agents respond via heuristics or rules of thumb of decision-making to handle immediate reactions to changes in their environment (e.g., food and perceived risk). Another good example is the "emotion system" of Giske et al.'s fish model (Giske et al., 2013), which integrates information, motivation, and physiological states in order to determine emotions, which in turn form the basis for "decisions" and subsequent behavioral outcomes. ABMs are especially suitable for answering ecological and evolutionary questions because they allow incorporating intra-specific variation, learning, and adaptation relatively easily, whereas inclusion of all of them in other model types was rarely, if ever, done. Akin to social systems (see below), ABM in ecology has moved towards convergence to some cognitive models, including the Fuzzy Cognitive Maps, social hierarchies (e.g., within primate troops (Cheney, and Seyfarth, 1992)) and neurobiological mechanisms, leading to the merger of population biology and behavioral ecology and the growing importance of neurophysiology as predicted by Wilson (1975).

3.2. ABM in social systems

In social systems, the importance of individual actions has also long been recognized as a critical driver of relevant processes (Ostrom, 2009; O'Sullivan et al., 2012, p. 113; Turner et al., 2003). The individuals in these systems, often embedded in various networks, are heterogeneous: depending on the objective of a certain project, agents could be entities at varying levels. For instance, cities are comprised of individual heterogeneous actors that are interconnected at multiple levels, which is analogous to organisms embedded in relevant hierarchical structures or networks (Batty, 2013). These heterogenous agents continuously interact with one another and with their environment. This emphasis on networks of individuals as a vital driver of social systems (Will et al., 2020) aligns well with broader changes in how cities (and other systems) are beginning to be viewed (Batty, 2013) .[1] Instead of distilling cities into homogeneous units whereby it was virtually impossible to say anything meaningful about the inner workings or micro dynamics (Batty, 2008), cities are now being viewed as dynamic organisms that are a product of networks, comprised of individual heterogeneous actors that are interconnected at multiple levels (Batty, 2013). The relationships between these actors are often non-linear, changing both spatially and temporally. When viewing a city in this way, the emphasis is on modeling, capturing, and replicating new emergent properties in a complex system comprised of individual components that evolve and interact.

Instead of a holistic approach to simulating social systems such as cities, aggregate mathematical approaches such as spatial interaction models (Batty, 1976) are still commonly used. Whilst the behavioral

[1] The United Nations predicts that by 2050 around 66% of the world's population will be living in urban areas. This expansion in urban populations will create significant challenges in creating sustainable and healthy cities with critical challenges needing to be met in improving water and transportation infrastructure, air pollution and waste management as well as provision of adequate housing, energy, health care, education and employment. This is just one example of the complex and multi-layered societal, economic and environmental challenges that governments and policymakers need innovative solutions to. While many models have been developed to address the impacts of future transport, housing or healthcare initiatives, most uses are purely empirical: they lack any consideration of the individuals and their actions and interactions that drive many of the processes behind these challenges.

foundations of these models are well understood (random utility, discrete choice models, etc.), more can be done to draw out the subtleties and detail of individual behavior and emergent social processes, especially in the context of increasing empirical evidence. In this context, mobile phone and social media data could give unprecedented insights into individual behavior, mobility, and their networks. Without an understanding of how these social processes play in shaping or affecting social systems dynamics, it is virtually impossible to verify any predictive simulation outcomes, i.e., to know whether the forecasts of how a social system will react to a specific impulse in the future are robust.

Despite new individual level data sets in abundance, considering and recognizing the importance of each individual, including the processes representing individual decisions and interactions as well as patterns that emerge from such processes, has been largely absent from many modeling efforts. ABMs can play an important role, representing both the individual and social processes when studying social systems and their emergence (Axelrod and Tesfatsion, 2006; Bae and Koo, 2008; Crabtree et al., 2017; Crawford et al., 2005; Crooks and Hailegiorgis, 2014; Makowsky and Rubin, 2013; Malleson et al., 2010). This is partially because ABM has the ability to embody the characteristics and behaviors of individual entities (e.g., humans, households), but can also capture system-wide emergent processes. ABMs bear the capabilities to model learning and adapting processes (An, 2012; Cumming, 2008; Milner-Gulland, 2012), and are thus able to explain or project macro-level features such as nonlinearity and thresholds, self-organization, uncertainty, unpredictability, surprising outcomes, legacy effects, time lags, and resilience (An, 2012; Levin et al., 2013, 2012; Liu et al., 2007). Consequently, social systems manifest features prevalent in many ACS (Liu et al., 2007).

Ecological modeling is not burdened with one of the major challenges in agent-based modeling as in social systems: representing human behavior (An, 2012; Groeneveld et al., 2017; Heckbert et al., 2010; Levin et al., 2013; Schlüter et al., 2017; Schulze et al., 2017; Verburg et al., 2016). Whilst agent-based modeling can adopt innovations from ecological modeling, which is already happening to some degree (Vincenot 2018), modeling human decisions and behavior remains a big challenge. Building on traditional simple optimization algorithms, progress has been made in cognitive frameworks for modeling human behavior, and examples include the beliefs, desires, and intentions (BDI) and the physical, emotional, cognitive, and social factors frameworks (PECS) (Conte and Paolucci, 2014; Schmidt, 2002). In the BDI framework, agents are endowed with a set of *beliefs* about their environment and about themselves, *desires* (expressed as computational states that are to be maintained), and *intentions* (computational states that the agents aim to achieve). Modeling human decisions and behaviors is becoming an area of increased research activity. For other approaches to modeling human decisions in ABM—such as microeconomic models, space theory-based models, and institution-based models—we refer to An and others (An, 2012; Groeneveld et al., 2017; Schill et al., 2019; Schlüter et al., 2017).

To date, agent-based models have proven successful as a tool for integrating knowledge across stakeholders to solve management issues, to understand co-evolution and emergent phenomena, and to address adaptive management issues called for by sustainability science. Examples are abundant, such as those in land use and land cover change (Groeneveld et al., 2017; Parker et al., 2003) and in common pool resource research (Poteete et al., 2010; Schulze et al., 2017; Seidl, 2015; Voinov and Bousquet, 2010).

3.3. ABMs in social-ecological systems

Social-ecological systems (SES) (Ostrom, 2009; Turner et al., 2003) also manifest the following features prevalent in many "pure" social or ecological systems according to Liu et al. (Liu et al., 2007) and others (Irwin and Geoghegan, 2001; Lindkvist et al., 2017; Malanson et al., 2006; Zvoleff and An, 2014): heterogeneity, reciprocal effects and feedback loops, nonlinearity and thresholds, surprising outcomes (observable as a result of human-nature couplings), legacy effects and time lags, and resilience (Levin et al., 2012; Liu et al., 2007). Synonyms of social-ecological systems include (complex) human-environment systems (An et al., 2020, 2005; National Research Council, 2014), coupled human and natural systems (CHANS) (Liu et al., 2007), and social-environmental systems (Schlüter et al., 2012a). Such systems are by nature complex adaptive systems, bearing properties of self-organization, uncertainty, unpredictability, and non-linear dynamics (Levin et al., 2012). The actors in these systems are heterogeneous, continuously interacting with one another and with their environment, learning and adapting (An, 2012; Cumming, 2008; Milner-Gulland, 2012). Computational models are exemplary tools for understanding social-ecological systems as complex adaptive systems, with the aim to increase our understanding of interactions, adaptive decision-making, co-evolution, and emergent phenomena (Schlüter et al., 2012b).

However, many challenges and possibilities remain in social-ecological sciences. To advance our understanding of social-ecological systems, more models need to explicitly be designed to focus on the feedbacks among actors and between actors and their environments. As with social systems, another challenge hinges upon modeling human decision-making and behavior. The methodological frontiers to address these needs include using patterns (or stylized facts) to validate model output and to guide parameter settings; using mixed methods approaches by including surveys, interviews, participatory modeling, and laboratory experiments to improve the representation of social-ecological systems and human behavior (Grimm et al., 2005; Heckbert et al., 2010; Schulze et al., 2017); and incorporating qualitative data. Finally, more transdisciplinary and interdisciplinary collaborations are key to increase the quality of models that address social-ecological systems because of the inherent interdisciplinary nature of research in these systems (Schulze et al., 2017).

A common real-world application of ABM in socio-ecological studies is to inform policy. To advance the use of ABMs for decision and management support, communication of model development, analysis, documentation, and presentation need substantial improvement towards more systematic and transparent ways (Heckbert et al., 2010; Müller et al., 2013; Schulze et al., 2017). ABMs have a potentially important role in normative institutional and policy "design" for social-ecological systems. Once researchers have empirically compelling representations of human behaviors in ABMs, one can test the extent to which a new proposed policy or design might result in adverse unintended consequences. For example, agent-based computational platforms for the exploration of new market designs for electric power systems are highly complex systems that involve intricate interactions among human, physical, and environmental agents. Traditional disciplinary boundaries (social sciences, engineering, physical sciences, etc.) are a major detriment for such "transdisciplinary" ABM application areas.

4. Traditional methods and models in ACS science

Different model types represent different tools, traditions, and basic assumptions about how systems under investigation work. Ideally, the perspectives represented by different model types are related to one another (Vincenot et al., 2016, 2011). Below we briefly review differences and complementarity between ABM and other kinds of models.

4.1. Weaknesses of non-ABM approaches in ACS

Traditional mathematical or analytic models are often based on a few simple equations or rules, including differential equations, dynamic state variable models, ideal free distribution models, game theory models, systems dynamics models, and statistical methods. To explain the complexity of ACS, such traditional mathematical or analytic models have shown a variety of strengths and weaknesses. Statistical models and system dynamics models are powerful in characterizing systems at an aggregate level, while lacking the ability to represent heterogeneous actors that interact with one another. Equation based and game theoretic models (Polasky et al., 2011) and system dynamics models are useful for representing feedbacks between systems, and for explaining macro-level characteristics, but lack the ability to represent the micro-level processes and interactions (Heckbert et al., 2010). Additionally, these methods cannot represent adaptive decision-making and the co-evolutionary aspect of ACS (except for Bayesian networks and evolutionary models), where a decision of one agent at one site or point in time may influence other agents' decisions, system events, and system level outcomes at different locations or later times. Thus, these non-ABM approaches fail in capturing the essence of ACS (Folke et al., 2010), which is problematic for improving governance and management strategies for increasing the sustainability of social-ecological systems.

In situations where interactions among agents are contingent on experience, and agents adapt to that experience, traditional equation-based models are often limited—if not impossible—for deriving the dynamic consequences. Traditional mathematical modeling approaches miss the capacity to handle some immediate (proximate) complexities that agents encounter, making it difficult to handle variation in individuals and their decision-making. In complex situations where agents have no experience, ABM scientists employ a range of useful techniques such as genetic algorithms and artificial neural networks, enabling agents to respond quickly and adequately (DeAngelis and Diaz, 2019). In such instances, agent-based modeling often offers the only practical method of analysis.

4.2. Complementarity and fuzzy boundaries with non-ABM models

Our exclusive focus on ABMs does not imply that we downplay, ignore, or even deny the important role of other types of models, in particular mathematical and statistical models. On the contrary, many ABMs (one type of mechanistic models) incorporate such types of models. ABMs do not replace but complement traditional mathematical or analytic models and they share many challenges in areas such as inverse parameterization, analysis of model robustness, coupling with traditional process-based models, and sensitivity and uncertainty analysis.

Moreover, the boundaries between ABM and traditional models are becoming porous: The majority of mathematical models are no longer solved analytically but numerically, which means that they are simulation models as much as ABMs. Consequently, many of the issues with ABMs reported here may also apply to mathematical modeling. Seppelt and Richter, for example, report on the solution of systems dynamics models: "We can show that solutions (a) differ if different development tools are chosen but the same numerical procedure is selected; (b) depend on undocumented implementation details; (c) vary even for the same tool but for different versions; and (d) are generated but with no notifications on numerical problems even if these could be identified" (Seppelt and Richter, 2005).

As discussed in the paper by Tesfatsion (2017), most agent-based models are not simply the computational implementation of a model or set of models previously developed in equation or whatever form. Rather, agent-based modeling often proceeds from agent taxonomy and flow diagrams, to pseudo code, and finally to software programs that can be compiled and run. In this case the software programs are the models. In principle, any ABM software program can decompose to—or equivalently be represented in abstract form as—a system of discrete-time or discrete-event difference equations, starting from user-specified initial conditions (Tesfatsion, 2017). However, these analytical representations become increasingly complex as the number of agents and rules defining their behavior increase.

4.3. Robustness analysis

"Robustness analysis" refers to building a set of similar, yet distinct, models of the same phenomenon, examining whether these models may lead to similar results despite their different assumptions, parameters, and/or even model structures (Levins, 1966). Robustness analysis was formulated for simple mathematical models but has recently been generalized for ABM (Grimm and Berger, 2016): different simpler versions of an ABM are created in the attempt to systematically break the models and thereby identify key mechanisms and limitations to explanations provided by an ABM.

Robustness analysis will help establish a new culture of communicating models: instead of only making sure that the model is realistic because it reproduces observations, we also need to demonstrate when and why the proposed mechanisms break down. The purpose of robustness analysis and related analyses is not only to obtain essential insights into the chosen study sites, but also about explicitly finding out what essential spatial, temporal, or organizational scales, what key processes/patterns, what feedback loops, heterogeneity, or tipping points/thresholds and so on may give rise to various aspects of complexity, including but not limited to emergence/surprising outcomes, resilience, and path dependence.

4.4. Coupling of ABM with other process-based models

Coupling ABM with traditional process-based models is an emerging research frontier in ACS research especially in earth system modeling and water resources system analysis. Among a set of major challenges highlighted in this domain (e.g., coupling ABM with other models, agents' decision rules, and spatial scale issues), how to fully address human behavior and its effect on the natural environment (such as irrigation, streamflow regulation and groundwater pumping) and dynamically capture the feedback of natural processes influencing human behaviors (such as climate change mitigation) to form a "tight" or "two-way coupling" (between ABM and process-based models) is a major challenge.

4.5. Handling uncertainty

As the agent-based modeling method matures, there are opportunities to begin to adapt useful methods from longer-established fields in order to improve the rigor of agent-based modeling. This is especially true with respect to how agent-based models deal with uncertainty. There are several reasons why uncertainty can make its way into model results. It might be a result of noise in the input data that are used to parameterize the model or because the model rules themselves are poorly specified (the model is not adequately representing the system that it is designed to represent). 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 (Murphy et al., 2004). The models are probabilistic, so naturally begin to diverge during the course of a simulation. By analysing the range of outcomes across an ensemble of models, it is possible to begin to better understand how uncertain the outputs are. Where most models are broadly in agreement in their results, there is less uncertainty compared to the situation where the models diverge substantially. One way to prevent a simulation from diverging from reality would be to occasionally incorporate more up-to-date data and adjust the model accordingly. There are a range of techniques that come under the banner of *data assimilation* that are designed for exactly this purpose. However, they have largely evolved from 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 (Clay et al., 2020; Long and Hu, 2017; Malleson et al., 2020; Rai and Hu, 2013, 2013; 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 are modelled. Consider the following example regarding the benefits of data assimilation approaches adapted from Swarup and Mortveit (2020). Agent-based modeling is an ideal tool to model disease spread, but typically models are restricted to hypothetical scenarios. However, with the abundance of new data that are available in near real-time, a high spatiotemporal resolution agent-based model of a national or global disease spread could be executed in real time, using data assimilation techniques to incorporate the most up-to-date disease surveillance data. The model could not only be used to make short-term predictions to highlight the emergence of potential new clusters, or as a virtual laboratory to test potential mitigation policies, but could also be used to highlight areas where its predictions are the least certain and would hence benefit from additional local data collection.

5. Challenges in agent-based modeling

The increasing recognition and application of ABMs in a wide range of disciplines should not warrant overlooking or downplaying the challenges that the ABM community needs to address in order to establish itself as a rigorous tool for advancing ACS science. These challenges, if not addressed with the highest priority in ABM research, can lead to *ad hoc* design of models which are nontransparent and untestable and, in turn, useless or even harmful for theory development and application in the long run.

Specifically, challenges abound in many aspects such as: (1) basic difficulties in model development, communication, understanding, verification, and validation; (2) difficulties regarding coherence because of the substantial variation in platforms, programming languages, model details and sophistication, and modeler's preferences, (3) difficulties in computational efficiency as most ABMs are developed on personal computers (but see these two papers (Tang et al., 2011; Tang and Bennett, 2011) for exceptions); (4) inadequate model/module transparency and reusability, which partially contributes to the challenge of verifying, validating, and analyzing model outcomes, including model sensitivity; and (5) difficulties in generalizing findings and scaling them across scales (An, 2012; An et al., 2005; Heppenstall et al., 2016; O'Sullivan and Manson, 2015; Parker et al., 2003).

We acknowledge that these challenges limit the usefulness of ABMs in scientific inquiry and empirical problem-solving domains. Nonetheless, it is worth pointing out that the basic principles of modeling, starting with a question and trying to find the right set of key processes of a system's internal organization, apply to any kind of mechanistic modeling. Consequently, the challenges to be mentioned below regarding communication, understanding, verification, validation, and so on are general and not specific for ABMs.

5.1. Integrated human-environment ABMs

The connections between human and environmental systems were assumed to be decomposable into a set of simple, unidirectional relationships, which has hindered understanding of these systems (An et al., 2014a). Many complexity features, e.g., those observed in several empirical social-ecological systems (Section 3.3), call for coupling of human and nature systems. In this context, researchers have proposed the coupled human and natural systems (CHANS) framework building on complex systems theory (Liu et al., 2007) (Section 3.3). However, there still exist many unanswered questions when people work under this framework: How do we customize the complexity of the representation of ecological and human processes to the intended purpose of the model (exploratory or theoretical/participatory/ descriptive or predictive)? How do the relative temporal scales of the ecological and human processes in the target system influence the representation of ecological processes (static/simple state transitions /dynamic), or influence the nature (e.g., tightness) of the coupling between ecological and human components of the model?

Building on a fundamental philosophy of methodological individualism, ABM has a unique ontology that represents key real-world actors as heterogeneous individual agents carrying attributes and actions (including interactions with other agents and/or their environment). This ontology allows a bottom-up style examination of many emergent outcomes that are prevalent in human-environment systems. ABMs are therefore very useful in modeling social-ecological (human-environmental) systems, given the complexity (nonlinearity and heterogeneity in particular) qualities that exist in these systems. For instance, ABMs should provide unique insights when modelers tackle issues around harmonizing social and environmental data that are subject to various spatial and temporal scales (extents/resolutions) or incorporate low-level processes and interactions within and between both dimensions of the CHANS system. Furthermore, ABMs provide a platform to perform policy or mind experiments or visualize outcomes under certain policy interventions.

5.2. Modeling human behavior

One hotspot research area is modeling human decision-making in ACS, especially decisions regarding their interaction with the environment. Here we refer to conceiving decision making at an individual level, rather than embedding it in social, institutional, and spatial contexts (O'Sullivan et al., 2012). Representing adaptive behavior is challenging in ABMs in general, including the behavior of cells in tissues, bacteria, plants, or animals because it has to be based on first principles, such as energy budgets (Martin et al., 2013), fitness seeking (Railsback and Harvey, 2002), photosynthesis (Scheiter et al., 2013), or stoichiometry (Sinsabaugh et al., 2013). Representing human behavior, however, adds further complexity because of social interactions in increasingly complex networks, anticipation of the behavior of others (which is addressed for simple settings in game theory), and memory, learning, and emotions, which all can lead to different decision "algorithms" in different contexts.

Current practice in representing human behavior is limited (Schlüter et al., 2017) and dominated by simple optimization algorithms. Moreover, there is no culture of rigorous theory development, which would require that alternative representations be implemented and tested for their ability to reproduce multiple patterns observed in real social systems. The key feature of this "pattern-oriented theory development" (Grimm and Railsback, 2012a; Railsback and Grimm, 2012) is that we would not strive to find a "perfect" representation of behavior of single individuals in simplified settings (such as in behavioral ecology and economics), but to select representations which are good enough to reproduce patterns observed at both the agent's and system's levels. Such tested representations should be referred to as "theories" of behavior and could constitute re-useable building blocks for representing human behavior in general. It is also expected, though, that different theories are needed in different contexts, so there might be no unique representation of human behavior. For example, during a panic in a theater, it is sufficient to represent humans as "Brownian agents", while in other contexts, we might need to include emotions and employ complex approaches such as neural networks and genetic algorithms to predict how agents respond to certain situations (Eliassen et al., 2016, 2009; Giske et al., 2014; Lindkvist and Norberg, 2014).

One of the hallmarks of ABM is its ability to capture and model human behavior; ironically, this is also one of the areas in which ABM has been heavily criticized (Heppenstall et al., 2016). Following the typology set out by Kennedy (2012), there are two broad ways to classify behavior: through mathematical or cognitive approaches. The mathematical approach centers on the custom coding of behaviors within the simulation, for example using random number generators to select a predefined possible choice (e.g., to buy or sell (Pumain and Sanders, 2013)). To understand human behavior in a more nuanced way–and to take account of factors such as individual preferences, local knowledge, and environment–developments of key things such as threshold-based rules are very important. These allow events to trigger a specific agent behavior for example, moving to a new location within a neighborhood (Crooks, 2010). These approaches have great utility when the behavior is both well understood and documented.

A second contrasting approach to simulating human behavior uses conceptual cognitive frameworks. Here, more abstract concepts such as beliefs, desires, and intentions (BDI) (Rao and Georgeff, 1991) or physical, emotional, cognitive, and social factors (PECS) (Schmidt, 2002) are embedded within individual agents. Both the BDI and PECS frameworks have been successfully applied to modeling human behavior within social sciences. For instance, for modeling the drivers of criminal behavior in an a-spatial model that uses the BDI framework, see Brantingham et al. (2005); for a geographically explicit model that represents behavior through the PECS framework, see Malleson et al. (2013)

Second, representing agents' decision-making processes in human-environment studies remains another major challenge. Here it is important to correct a major misconception still being expressed by some commentators uninformed about the powerful capabilities of modern software: namely, the misconception that ABM representations of human decision-makers must necessarily be "stupid". To the contrary, the constraints on agent decision making implied by ABMs are constraints inherent in every real-world social system. The decision-making representation methods used by ABM agents can range from simple behavioral rules to decentralized optimization to sophisticated anticipatory learning algorithms for the approximate achievement of intertemporal objectives.

A framework for mapping and comparing human decision making in models of socio-ecological systems, dubbed MoHub (Modeling Human Behavior), has recently been published (Schlüter et al., 2017) with the aim to facilitate choices of how to model human decision making. This is important because of the strong impact assumptions on human behavior may have for model outcomes and its final impact on e.g., policy recommendations.

5.3. ABM transparency and reusability

Lack of transparency and reusability in ABM code has been mentioned as one of the bottleneck problems for the ABM community (An et al., 2014a; Evans et al., 2013; National Research Council, 2014; Parker et al., 2003). Part of this problem stems from a lack of central development within ABM. ABM has a somewhat fragmented development with advances being made in different disciplines, for example validation approaches in ecology (Grimm et al., 2005), and handing of space in geography (Heppenstall et al., 2016). Without adequate transparency and reusability, it is not only very difficult to verify and validate ABMs, but a large amount of resources are wasted, such as modules and programming libraries that have been developed and tested by ABM experts and could have been reused. In human dynamics research, the lack of open source software packages has become a major impediment to the promotion of ABM. The availability and widespread use of source codes will play a critical role in the adoption of new perspectives and ideas enhancing ABM. More toolkits are needed to interface the open source revolution and ABM, seeking cross-fertilization between these two fast-growing communities.

There are, though, initiatives to tackle the challenge of documenting and presenting agent-based models. Fortunately, the development of presentation protocols for ABM is now an active area of research. Grimm et al. developed the Overview, Design concepts, Details (ODD) protocol as a standard format for describing ABMs in ecology and beyond (Grimm et al., 2020b, 2010, 2006). It provides a fixed structure and terminology, making model descriptions start with an overview of the model's purpose, entities, state variables, scales, and processes and their scheduling, followed by listing how important design concepts for ABMs, such as emergence or interactions, have been considered. Finally, details on initialization, input data, and all process representations (submodels) are given. The purpose of ODD is to facilitate reading and understanding, to provide exactly the same kind of information always in the same sections, and to provide all details that are needed for re-implementing the model.

The use of the ODD has improved transparency in ABM, but limitations remain because verbal model description will always include ambiguities (Grimm et al., 2020b). Moreover, for specific classes of models, a more refined structure might be useful. This is in particular the case for modeling human behavior. Therefore Müller et al. suggested ODD + *D*, adding elements that facilitate selecting and documenting important features in models of human decision making (Müller et al., 2013). Some scholars have criticism for applying ODD to ABMs in all situations, but suggest development of multiple standardized presentation protocols, which should be tailored to the purpose and development of a modeling effort.

Reusability is fostered by archives of existing models which include not only the program code but also instructions for use and transparent model descriptions, preferably using the ODD protocol. The Model Library of CoMSES.net has become a useful platform where modelers can seek building blocks to incorporate in their own models; it even provides a database with all agent- and individual-based models published so far. NetLogo (Wilensky, 1999), specifically designed for ABMs and increasingly used for implementing ABMs, is easy to learn (Railsback and Grimm, 2012; Wilensky and Rand, 2015) and computationally less limited than generally believed (Railsback et al., 2017). Another route to reuse of models is model re-implementation. Instead of starting each modeling project from scratch, Thiele and Grimm suggest to scan existing models and try and re-implement the most suitable one (Thiele and Grimm, 2015). Even if the final model only includes a few elements of the re-implemented model, starting from an existing model saves a considerable amount of time for model formulation, which then can be invested in model analysis and improvement. Re-implementation also fosters theory development, because researchers can try and break models to identify elements and processes that are essential for the model to produce realistic results. Computational modeling in general needs to go beyond showing that a model looks right by showing where and when they go wrong (Grimm and Berger, 2016; Thiele and Grimm, 2015).

5.4. ABM verification and validation

Verification and validation of ABMs has been a problem besetting ABM modelers and users for many years (An et al., 2014b, 2005; Manson, 2002; National Research Council, 2014; Parker et al., 2003). Many issues arise from this difficulty (Couclelis, 2002), although this problem is not confined to ABM—it also besets other domains of modeling. For instance, the global climate research community is struggling with the credibility of different General Circulation Models when they cannot reproduce the historical climate. Without robust model validation and a joint understanding of what model validation and verification is, the reliability of ABM cannot be established, limiting its usefulness and application in various contexts (An et al., 2014b; Brown et al., 2008).

Augusiak et al. reviewed terminology regarding the term "validation" and came to the conclusion that this term cannot be used for any practical purpose anymore, because it is impossible to boil down its wildly varying definitions and interpretations to a single one (Augusiak et al., 2014). As a solution, they suggest the artificial term "evaludation" (a merger of "evaluation" and "validation"), which covers all elements of iterative model development: model purpose, conceptual model, data evaluation, software verification, model output verification and corroboration, and model analysis. They then point out that the general notion of "validation" often is too narrow, requiring that, as in physics, a model makes predictions of features that were not used for model calibration, i.e., independent, or secondary, predictions. It is thus important to distinguish between model verification, which shows that the model reproduces calibration patterns, and model "corroboration", which is about independent predictions. Documenting how all these elements were addressed during model development is facilitated by using the standard documentation format TRACE (Grimm et al., 2014).

Empirical validation of ABMs is a highly active research area. As discussed in Tesfatsion's paper (Tesfatsion, 2017), ABM permits model-builders with scientific objectives to strive for the simultaneous achievement of four distinct aspects of empirical validation, i.e., 1) *input validation:* Are the exogenous inputs for the model empirically meaningful and appropriate for the purpose at hand? 2) *process validation:* How well do the physical, biological, institutional, and social processes represented within the model reflect real-world aspects important for the purpose at hand? Are all process specifications consistent with essential scaffolding constraints, such as physical laws, stock-flow relationships, and accounting identities? 3) *descriptive output validation:* How well are model-generated outputs able to capture the salient features of the sample data used for model identification? And 4) *predictive output validation:* How well are model-generated outputs able to forecast distributions, or distribution moments, for sample data withheld from model identification or for data acquired at a later time or a different place?

This pursuit of comprehensive empirical validation will of course be tempered in practice by data limitations. Even in an era of big data and data advances, data availability and quality remain important concerns. Computational limitations such as round-off error, truncation error, and error propagation also remain a concern. Fortunately, advances in computer technology and numerical approximation procedures are rapidly reducing these limitations.

5.5. Big data and high-performance ABM

This potential of ABM's capacity to leverage big data is improved by the increasing availability of big data such as high-resolution remote sensing imagery, social media data, and large, detailed human socio-economic datasets (Wang et al., 2013; Ye and He, 2016). Big data are characterized by their characteristics in terms of volume (size of data), velocity (update frequency), variety (types of data), veracity (quality of data), and value (importance). Currently ABMs are largely based on data from relatively small or local scales, limiting the usefulness of ABM in large (spatial extent) and high-resolution contexts—for a small set of exceptions that use parallel computing, see the work by Tang and associates (Tang et al., 2011; Tang and Bennett, 2011).

While there is a growing use of agent-based models for a variety of applications, there are several key challenges that need to be overcome. These range across the spectrum from theory to practice and from hypothesis to application (Crooks, 2010). However, the greatest challenge to ABM is akin to many other modelling methodologies, in that the realism that an ABM can bring to a simulation is highly dependent on the quality of the data that it uses (i.e., veracity for big data). Agents require accurate individual-level behavioural data if they are to produce simulation results that can be used for policy. Without rigorous calibration (fine tuning the model) and validation (testing the model on unknown data) of the ABM, any outputs are essentially meaningless. A typical ABM can include hundreds to millions of heterogeneous agents each operating their own individual rule sets–calibrating and validating these models with stochasticity therefore requires a huge amount of individual level data and leads to massive intermediate or output data (e.g., based on considerable Monte Carlo runs). In other words, even if the spatial extent of an ABM is not large, the modelling steps (from verification, calibration, validation, to experimentation) can easily pose a big data-driven challenge.

Fortunately, "big data" can potentially provide the level of detail required. The term "big data" is somewhat misleading, which refers to both traditional large data sets, for example national censuses, as well as new digital information generated from social media, high resolution satellite imagery, gene sequencing data, and the like. With the proliferation of social media, information generated and disseminated from these outlets has become an important part of our everyday lives. Our ways of examining social-spatial interactions are increasingly transformed by the development of more powerful computing technologies, emerging big and open data sources, and new perspectives on social-spatial processes (Shaw et al., 2016). Social media, such as Twitter, capture data about individual behavior and movements that have previously been absent from modelling efforts (e.g., considering the veracity issue). As more social media data are increasingly available, agent-based modelling has been used to predict human behavior like posting, forwarding or replying to a message with regard to topics and sentiments (Ye and Lee, 2016). Despite the obvious potential of "big data", there are considerable issues to overcome such as bias, noise, generalization and in some cases, the ethics of whether researchers should be using this kind of data (Heppenstall et al., 2016).

To resolve the big data and computing challenges facing ABMs, high-performance computing enabled by state-of-the-art cyberinfrastructure represents a unique solution. A series of ABMs based on high-performance computing have been reported in the literature (Tang et al., 2011; Tang and Bennett, 2011; Tang and Jia, 2014). High-performance ABMs often focus on large spatiotemporal extents and/or fine resolutions (Tang and Jia, 2014). Large-scale ABMs rely on two typical parallelisms, message-passing and shared memory (Wilkinson and Allen, 2004), which allow for dividing (e.g., via spatial domain decomposition (Ding and Densham, 1996; Wang and Armstrong, 2003)) a model into smaller sub-models that can be deployed to high-performance computing resources for parallel computing (Tang and Wang, 2009). Message-passing, shared-memory, or the combination of both enables the inter-processor communication for data or information required by neighbouring sub-models (Gong et al., 2013; Shook et al., 2013). This high-performance computing solution is not only suitable for ABMs with large spatiotemporal extent and fine resolutions, but also can facilitate the use of small-scale ABMs in need of huge computational support. These small-scale ABMs often require a significant number of Monte Carlo repetitions through alternative modelling phases, including calibration, verification, validation, sensitivity and uncertainty analysis, and experimentation for scenario analysis. These massive Monte Carlo runs, while independent of each other, can be deployed to, and thus accelerated by, high-performance computing resources (Tang and Bennett, 2010).

5.6. Spatially explicit ABMs

There are many modeling issues that apply to, but are not limited to, spatially-explicit models, e.g., the effects of random number generators; the way to handle boundary conditions; the effects of spatial structure and model type on ABM evaluation (e.g., via sensitivity analysis); the effects of spatial resolution, extent, and data on model calibration and validation; and the possibility and benefits of employing alternative spatial representation (in comparison to the traditional Cartesian space)—e.g., adoption of relative space in ABM (An et al., 2015). Informed decisions on these issues may be conducive to developing more robust ABMs. We refer readers with interest in this domain to Manson et al. (2020).

Finally, the above challenges are also affected by the spatial scale issue of ABM setup. ABMs are often developed with an implicit assumption that agents interact with each other within a system. However, agents across distant systems around the world have rarely been taken into consideration even though they are increasingly interacting. To understand and manage such complex distant interactions, an integrated framework of telecoupling has been developed (Liu et al., 2013) (http://telecoupling.org). Telecoupling is defined as socioeconomic and environmental interactions between multiple social-ecological systems over distances. As an umbrella concept, it encompasses many processes, such as migration, trade, tourism, species invasion, environmental flows, foreign direct investment, and disease spread. Telecouplings have profound implications for global sustainability and human well-being as they can transform the structure, function, pattern, process, and dynamics of social-ecological systems across local-to-global scales. Thus, it is necessary to develop a new set of ABMs–Telecoupled Agent-based Models (Liu et al., 2014).

6. Opportunities from artificial intelligence and data science

The challenges summarized in Section 5 not only limit the usefulness of ABMs in scientific inquiry and empirical problem-solving domains, but also hamper our understanding of ACS structure and processes. Fortunately, the advances in artificial intelligence, unique new forms of data, and data science will substantially help address these challenges.

6.1. Opportunities from artificial intelligence

Starting in the l950s, modern artificial intelligence (AI) has aimed to emulate the 'natural' intelligence seen in human or animal behavior under a critical assumption that, to a large degree, machines can be made to simulate human intelligence. Typically, this means being able to demonstrate cognitive functions usually displayed by humans such as goal-oriented behavior, learning, reasoning, knowledge representation, planning, language processing, and problem solving (such as the ability to move and manipulate objects by, e.g., robots).

AI is also an academic discipline for its own right, albeit one that is highly fragmented. AI leverages both traditional (e.g., statistical methods, mathematical optimization, economics) and non-traditional methods (e.g., artificial neural networks, computational intelligence) to understand and simulate human intelligence. Sub-disciplines of AI range from those associated with the use and development of statistical techniques such as regression to recognize patterns in data, to the creation of human-like intelligent robots that are able to perceive their environment and learn to conduct particular tasks (e.g., recognizing an object and interacting with it).

Considering the goals and methods of AI, AI appears a natural solution for the ABM challenges described above. Although the ability to create truly 'intelligent' agents is obviously extremely relevant to ABM, most agent-based models do not actually require agents with such a high degree of intelligence. The contribution of AI to ABM is most keenly felt by developments that are more commonly used in data science such as machine learning: regression, neural networks, reinforcement learning, etc.

However, progress has been slower than expected, with data limitations being one of the most fundamental reasons. As most AI methods that could be employed to build 'intelligent' agents require large amounts of (often individual level) data, and such sources were not readily available in the past. Alongside the methodological developments that are emerging under the banner of AI, there has been another transformative change that has fostered the success of AI-related developments and is directly relevant to ABM: the emergence of big data.

6.2. Opportunities from big data

The advent of big data may provide a solution for using AI to nourish ABMs. The usefulness of big data should be highlighted in understanding agent-based complex systems. As noted, we have increasing amounts of individual level data, but a challenge remains in how to link disparate data sets and extract useful information and insights offered by these data. It is not only burdensome in obtaining, storing, cleaning, or mining such new forms of data, but there are also ethical problems with sources such as GPS telemetry, social media, and remote sensing, when we aim at revealing detailed information about individual actions or local processes. Furthermore, it may be more challenging to resolve biases from big data than from carefully crafted traditional data. The majority of published applications use more traditional data types, which is most likely due to the fact that modelers are more comfortable with manipulating traditional sources of data (e.g., census data, various sample data (Robinson et al., 2007)) rather than mining new forms of data, or consider these new sources of data as too noisy, biased, or inaccurate.

Despite these challenges, big data may provide us with new avenues with which to explore how people perceive, use, and react to events in the spaces around them, and the potential to incorporate these observations into our models in near real time. Moreover, many of these sources of data allow us to examine 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.

Such data (micro-data mostly) driven models, including ABMs, may suffer from a serious drawback: they are heavily data-driven or data-centered with little consideration of theory. As a result, it is almost impossible to reproduce model results or to interpret them. For instance, Othman et al. created an ABM of the rail network in Singapore, which used only train ticket purchasing data as its input (Othman et al., 2015). There is an implicit assumption that models built using new forms of micro-data will capture the essential processes that are taking place in these systems. However, ABMs that represent dynamical processes as snapshots in time can be misleading (Hassan et al., 2008). This leads to another weakness of many micro-data driven models: without actually knowing much about the important processes that need to be captured, it is an almost impossible task to build models that are representative of the "real" world and generate meaningful results. Yet modern data science, especially combined with artificial intelligence, may help substantially address this challenge.

6.3. Opportunities from qualitative data

Another prominent issue is the lack of using qualitative data, particularly ethnographic data (such as text, images, videos, and audio documents) in ABM (Agar, 2005); for exceptions see the work by Lindkvist et al. and Schulze et al. (Lindkvist et al., 2017; Schulze et al., 2017). This trend matches the basic idea of "pattern-oriented modelling" (Grimm et al., 2005; Grimm and Railsback, 2012b; Railsback and Grimm, 2019) where a combination of several qualitative (or "weak") patterns, which a model is supposed to reproduce, can be as effective or even more so than using a single, highly detailed pattern to reject unsuitable submodels and parameter combinations. A typically weak, but still quantifiable, pattern refers to a situation in which certain variables—for example population size, average wealth, average and higher moments of age, or time needed to recover from a disturbance event—stay within certain intervals.

An emerging literature has noted that ethnography can be systematically used to inform both functions of social processes and decision making rules within ABMs, provide insight into selecting outcome variables for analysis, increase ABM quality and empirical accuracy—especially in representing human decision making and social systems (Tubaro and Casilli, 2010). For instance, the Modelling Agent systems based on Institutional Analysis framework (MAIA) has been used for participatory ABM development with ethnographic data (Ghorbani et al., 2015). Although Yang and Gilbert developed guidelines for ethnographically informed ABMs, there remains a need to more broadly apply and refine both the MAIA framework and modeling guidelines (Yang and Gilbert, 2008).

Increasing the use of qualitative data is challenging as few researchers are competent in both ABM building and qualitative ethnographic data collection and analysis (Tubaro and Casilli, 2010). Addressing this challenge requires either training new interdisciplinary ABM researchers or increasing collaboration among quantitatively and qualitatively trained researchers. Further, qualitative data are often seen as "lacking rigor" and there is a need to bridge the cultural gap between

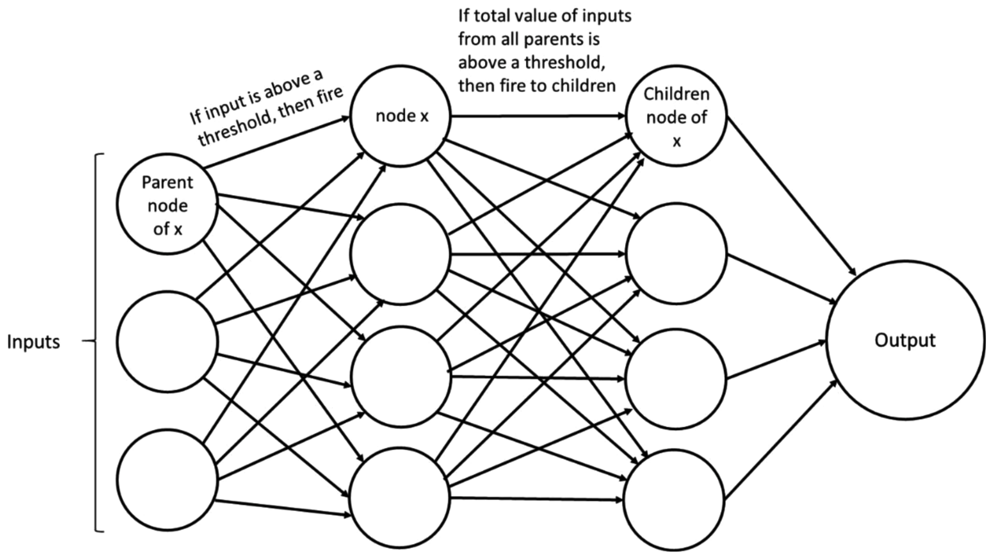

Fig. 3. Structure of neural network.

quantitative and qualitative researchers. Regardless, agent-based modelers and qualitative researchers share the overlapping goal to understand mechanisms and processes in social systems (Yang and Gilbert, 2008), making increased collaboration a compelling means to strengthen ABMs' representation of the system(s) and social processes.

Methodological challenges arise in areas such as translating qualitative data to quantitative model parameters and model generalization from inherently context-specific ethnographic data. When extracting patterns and identifying thresholds or multipliers from qualitative data such as field notes from participant observation, there will inevitably be instances of "unjustifiable, 'magic' constraints in the code" (Yang and Gilbert, 2008, p. 7). Further, there will be places where the code must be made more precise or concrete than the context of the qualitative data would allow. When faced with the challenge of defining parameters based on qualitative data, the most important consideration is not the specific numbers, but on whether the numbers can reproduce or represent the patterns identified in the qualitative data. Then, as with any ABM, the impact of parameter variations should be addressed via sensitivity analysis and discussed in the context of the ethnographic case, or ideally, cases (Yang and Gilbert, 2008).

6.4. Opportunities from data science

The field of data science refers to the use of scientific methods, programming tools, and appropriate data infrastructures to derive insight from data that can lead to a better understanding of some underlying phenomena. Successful data science methods or techniques are emerging in many areas of research or empirical applications. For example, convolutional neural networks (CNNs) have demonstrated success in classifying or segmenting hyperspectral satellite imagery (Ma et al., 2019) and detecting targets from aerial vehicle imagery (Vidal-Mata et al., 2020). Recurrent neural networks (RNNs) have been a popular option for time series forecasting, with vast applications ranging from modeling COVID-19 transmission (Chimmula and Zhang, 2020) to upcoming earthquake prediction. Graph neural networks (GNNs) recently emerged to model predictive tasks defined over a graph or a network (Kipf and Welling, 2016) such as to capture the complex spatial patterns underlying graph-structured geospatial data (Zhu and Liu, 2018), or to model the information propagation or event prediction in a social network (Fan et al., 2019).

Many above data science techniques, with essential contribution from artificial intelligence, data analytics, and high-performance computing, can be extremely valuable as a means of deriving insight from data to inform the basic structure of a model (i.e., to provide empirical support for underlying theories), as well as to calibrate and/or validate agent-based models. Crooks and Wise demonstrate how crowdsourced spatial data can be used to better understand the real-world situation after a humanitarian crisis and use that new information to inform an agent-based model to support relief efforts (Crooks and Wise, 2013). Similarly, Crols and Malleson use real-time footfall data, coupled with an agent-based model, to estimate the demographics of visitors to a town center (Crols and Malleson, 2019). Even deep generative models have been introduced to synthesize high-fidelity data samples with realistic representations of the underlying spatial correlation structure for GIS applications (Klemmer et al., 2019). Below we briefly review two kinds of machine learning.

Machine learning via regression: In addition to providing a means to generate data that can be used to calibrate and validate agent-based models, big data and associated data science techniques can also be used to improve the behavior of agents. One of the most well-known data science techniques is machine learning (ML). As a subfield of artificial intelligence, ML refers to a suite of algorithms that have a generic structure but can be parameterized to detect relationships in data through a process of "training". Specifically, ML extracts patterns and learns accurate predictive models, from (often) massive data, without being explicitly programmed—put another way, ML learns a predictive function from data. Training involves feeding data to the algorithm so that it can estimate the parameter values that best allow it to distinguish between different patterns in the data. 'Supervised' ML algorithms are provided with data that have already been labeled, so the aim of the training process is to identify which input values lead to a given output. Probably the most widely used supervised machine learning technique is linear regression. A regression equation typically has the form:

$$y = \alpha + \beta_1 x_1 + \ldots + \beta_n x_n + \epsilon$$

where y is the dependent variable to be predicted and $x_1 \ldots x_n$ are the independent variables. The model is trained with data so that the parameters α and β_s ($s = 1, 2 \cdots$ n) can be estimated. In that way the generic model structure can be parameterized to detect relationships in vastly different data sets. Regression equations are commonly used to better understand a particular phenomenon–e.g., to provide empirical support for a given theory–and use this information to inform an agent-based model, but they can also be used directly to control the behavior of the agents. For example, Zhang et al. present an agent-based model of solar panel adoption that includes agents whose behavioral choices, rather than being programmed directly, are determined through the application of a regression model (Zhang et al., 2016).

*Machine learning via neural net*works: In recent years, more advanced machine learning techniques have evolved to model non-linear patterns that cannot be represented by standard regression techniques. Of these, neural networks have emerged as one of the most versatile algorithms. A neural network consists of layers of nodes that are connected by links (Fig. 3). As input data are fed into the algorithm, nodes receive messages from parent (i.e., message sending) nodes and 'fire' messages to their child (message receiving) nodes depending on whether the messages that they receive as input are greater or lesser than some threshold. Like a regression equation, these thresholds are parameters that need to be optimized. A process called 'back-casting' allows the neural network to estimate optimal values for these parameters from training data.

Neural networks were inspired by the structure of the brains of animals, so are of obvious interest to agent-based modelers. It is feasible that rather than attempting to define decision rules for agents by hand, each agent could be implemented with their own neural network in a similar way to Zhang et al.'s agents who had their own regression equations (Zhang et al., 2016). Then the process of calibrating the model would involve optimizing the neural networks for all the agents. However, the uses of neural networks to control the behavior of agents directly are relatively rare. This could be because the process of calibrating a model could be extremely difficult: a single neural network typically requires very large volumes of training data, so a model that consists of large numbers of independent neural networks (one per agent) would be very challenging indeed. Or perhaps they are not seen as attractive because it is very difficult to interpret *why* a neural network makes its predictions.

A GNN typically learns node representations by recursively aggregating information from their neighborhood nodes. Classical GNN tasks include graph classification, e.g., molecular structure classification (Ying et al., 2018), node classification (e.g., publication classification in an article network (Karimi et al., 2019; Kipf and Welling, 2016), link prediction (e.g., predicting integrations in a social networks (Zhang and Chen, 2018)), and collaborative filtering (e.g., recommendation systems like Amazon or Netflix (Wang et al., 2019)). Most population-level interactions come naturally in the form of graphs and can be modeled as graph edges. For example, in geospatial data, spatial objects can be represented as nodes and their topological/attribute relationships are represented as links, making GNNs the natural model choice. Furthermore, GNNs can be cascaded with other models such as CNNs, for joint information extraction on the individual level (though CNNs or so), and interaction modeling on the population level (through a GNN). Furthermore, GNNs can be cascaded with other models such as CNNs, for joint information extraction on the individual level (though CNNs or so), and interaction modeling on the population level (through a GNN).

A concrete example of using GNNs to derive behavioral rules of networked entities can be found in a recent application in the autonomous flocking of multi-agent robot swarms. The authors consider a decentralized network of moving robot agents: each agent is viewed as a node in a dynamic graph with two agents within a communication range connected by an edge, and changes in this one graph are determined by both GNN and RNN**.** A GNN is applied on top of the graph for aggregating and forecasting the population-level behavior patterns. Further, each individual agent (node) can perceive the visual environment and extract features by its own convolutional neural network (CNN), which processes each drone's visual input like "eyes". Note that each node or agent has its own CNN. The resulting model is then a CNN-GNN stack and can be trained from end to end.

Similar ideas can be potentially extended to handling any dynamic network with semantically rich nodes, such as forecasting COVID-19 transmission by exploiting the multimedia information from a social network, where people are the nodes, and person-person contacts are the links that change over time. This would enable modelers to use a unique RNN for each agent and model each person's (nodes) health status over time. An RNN can be a naïve baseline itself, without considering population influences, while a GNN can be used to model the population-level interactions (edges) that change over time too.

6.5. *Agents learn and form behavior*

One area where neural networks are offering a promising route forward is through allowing agents to learn about their environment for themselves. A valuable feature of an agent-based model is that the behavior of agents can tell us something about the underlying system, but we lose this advantage if the agents themselves are black boxes and we cannot understand why agents make decisions as they do.

We can better understand why agents make their decisions through methods such as *reinforcement learning*, where positive behaviors are "learned" through repeated exposure to an environment through building and refining deep neural networks. Such networks may capture uncertainty and incomplete knowledge representations. With large-scale individual tracking data, it may be possible to teach agents how to navigate spaces as if they were humans. These 'learning' agents may both better reflect the actual behaviors of humans and model their behavior under changing conditions. Progress is rapidly being made elsewhere (Banino et al., 2018), but integration into geographical modelling remains a challenge (but see, e.g., work by Abdulkareem et al. (Abdulkareem et al., 2019) using Bayesian Networks to help simulate complex decision-making with regards to potential cholera infection).

Agent behavioral learning can also happen with the aid of big data. For instance, with time series data of particles' mass, charge, and geographic positioning information data, GNN can be trained to derive closed-form, symbolic expressions of Newtonian force laws and Hamiltonians (Cranmer et al., 2020). The authors begin with a starting graph (say with n_1 particles and n_2 edges describing their relationships). The authors use 1) <u>an edge model</u> to represent links/edges among all n_1 particles—here is the key of their work: there are many potential equations (they aim to find them by GNN; they are expressed as inductive biases), which represent potential math functions of Newtonian force laws. Here the goal is to use GNN to select function type and fine-tune the value of all parameters in the corresponding function (say one of the functions is named f_1). Then, the authors use 2) <u>a node model</u>, in which each node (particle) receives all the messages from all the rest (n_1–1) of the particles with the magnitude of each message (i.e., amount of gravity) calculated from the candidate function (say f_1). The authors use 3) <u>a global model</u> to aggregate and update the status of all messages and nodes over time.

Below is the selection process: Once a GNN-based function (e.g., f_1, plus number of parameters as part of complexity) is used, the authors calculate the status of all particles and compare them to the observed data of these particles (i.e., the time series of particle data or spatial panel data mentioned at the start of this text). A certain measure (normalized mean square error or NMSE) is used to choose among the different alternative functions (plus parameter values) with model complexity (number of parameters and operators) in control. The authors use the Occam's razor rule to choose the final function (or symbolic regression outcome): when the NMSE is large, the same, or close, one with the least amount of complexity is the winner. Finally, the authors found that the symbolic closed-form model derived from ML is what Newtonian force laws express.

7. Significance

This article aims to air critical state-of-the-art ABM issues and provide a venue to seek resolutions. First, we bring several compelling ABM problems and challenges to the forefront at the right timing with insight from key community leaders and practitioners. At a time in which the use of ABMs is exploding, but maintains a series of unresolved challenges, this paper has used input from around 100 exceptional scientists

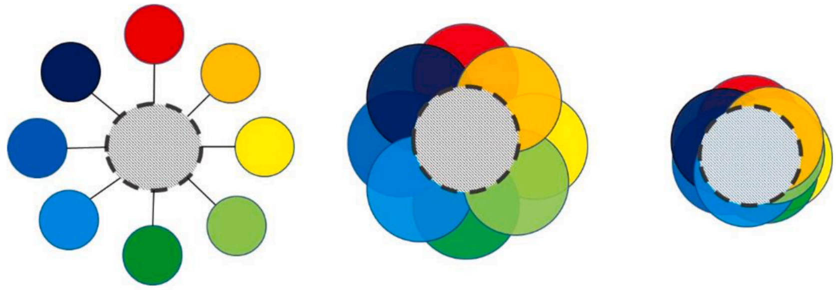

Fig. 4. Paradigm shift from multidisciplinary (A), to interdisciplinary (B), to transdisciplinary research (C) in ACS Science. The dashed circle in the center stands for the subject under research, and different colors for different disciplines (http://www.ed-archmat-ejd.eu/index.php/vision-aims.html).

with very diverse backgrounds (http://complexities.org/ABM17/), to depict the state-of-the-art about ABMs, providing inspirations and directions for many related fields. To break new ground, we have developed a set of guidelines for modelers and reviewers and for novices (See supplementary information). At the same time, we provide a comparison of commonly used ABM toolkits and software packages given the existence of 85 + platforms or toolkits for ABM, and recommendations for ABM/ACS education (See supplementary information). Furthermore, we provide a review of the use of ABM in coping with COVID-19 challenges.

This article is not only a pile of papers, facts, strengths, and challenges related to ABM, but also aims to provide new insights into the field of modeling ACS, point out impending tasks, and envision long term directions of ACS studies. In the short term, we show the huge opportunities provided by data science and artificial intelligence (Section 6). In the long run, we call for an AI-informed ACS science, which warrants a transdisciplinary approach. Under the transdisciplinary approach, all relevant disciplines are fused more seamlessly to detect and express mechanisms that have generated macro-level outcomes (Fig. 4). Historically, science benefited from the so-called multidisciplinary approach (Fig. S4A), which features a concurrent, parallel investigation of the same phenomena or subject from many relevant disciplinary perspectives or an integration of them (Conte and Paolucci, 2014). An advance in scientific inquiry is to invest in interdisciplinary efforts, which aim to interweave knowledge, theory, and methods from many relevant disciplines, performing multilevel and modular modeling (Fig. S4B). Under transdisciplinary efforts, artificial intelligence, data science, and domain knowledge will be interweaved to generate pathways or mechanisms that are more meaningful, effective, and less error-prone in understanding and envisioning ACS (Fig. S4C).

With a clearer picture of ABM strengths, weaknesses, available resources, and impending tasks and future directions, more potential users or developers, and even commercial companies, will be attracted to engage more with the ABM community, allocating necessary resources to the science, technology, and application of ABM, enhancing ABM software and capabilities.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.ecolmodel.2021.109685.

References

Abdulkareem, S.A., Mustafa, Y.T., Augustijn, E.-.W., Filatova, T., 2019. Bayesian networks for spatial learning: a workflow on using limited survey data for intelligent learning in spatial agent-based models. Geoinformatica 23, 243–268.
Agar, M., 2005. Agents in living color: towards Emic agent-based models. J. Artif. Soc. Soc. Simul. 8.
An, L., 2012. Modeling human decisions in coupled human and natural systems: review of agent-based models. Ecol. Model. 229, 25–36.
An, L., Grimm, V., Sullivan, A., Turner II, B.L., Wang, Z., Malleson, N., Huang, R., Heppenstall, A., Vincenot, C., Robinson, D., Ye, X., Liu, J., Lindvist, E., Tang, W., 2021. Agent-based complex systems and agent-based modeling. Work. Pap. Cent. Complex Hum.-Environ. Syst. San Diego State Univ. URL http://complexities.org/Photo&PDF/ACS-ABM-document.pdf.
An, L., Linderman, M., Qi, J., Shortridge, A., Liu, J., 2005. Exploring complexity in a human-environment system: an agent-based spatial model for multidisciplinary and multiscale integration. Ann. Assoc. Am. Geogr. 95, 54–79.
An, L., Mak, J., Yang, S., Lewison, R., Stow, D., Chen, H.L., Xu, W., Shi, L., Tsai, Y.H., 2020. Cascading impacts of payments for ecosystem services in complex human-environment systems. J. Artif. Soc. Soc. Simul. 23, 5.
An, L., Tsou, M.-.H., Crook, S., Chun, Y., Spitzberg, B., Gawron, J.M., Gupta, D., 2015. Space-time analysis: concepts, quantitative methods, and future directions. Ann. Assoc. Am. Geogr. 105, 891–914.
An, L., Zvoleff, A., Liu, J., Axinn, W., 2014a. Agent based modeling in coupled human and natural systems (CHANS): lessons from a comparative analysis. Ann. Assoc. Am. Geogr. 104, 723–745.
An, L., Zvoleff, A., Liu, J., Axinn, W., 2014b. Agent based modeling in coupled human and natural systems (CHANS): lessons from a comparative analysis. Ann. Assoc. Am. Geogr. 104, 723–745.
Arthur, W.B., 1999. Complexity and the economy. Science 284, 107–109.
Augusiak, J., Van den Brink, P.J., Grimm, V., 2014. Merging validation and evaluation of ecological models to 'evaludation': a review of terminology and a practical approach. Ecol. Model. 280, 117–128.
Axelrod, R., Cohen, M.D., 1999. Harnessing Complexity: Organizational Implications of a Scientific Frontier. The Free Press, New York.
Axelrod, R., Tesfatsion, L., 2006. A guide for newcomers to agent-based modeling in the social sciences. In: Tesfatsion, L., Judd, K.L. (Eds.), Handbook of Computational Economics: Agent-Based Computational Economics. North-Holland Publishing Co., Amsterdam, Netherlands, pp. 1647–1659.
Bae, J., Koo, J., 2008. Information loss, knowledge transfer cost and the value of social relations. Strateg. Organ. 6, 227–258.
Banino, A., Barry, C., Uria, B., Blundell, C., Lillicrap, T., Mirowski, P., Pritzel, A., Chadwick, M.J., Degris, T., Modayil, J., Wayne, G., Soyer, H., Viola, F., Zhang, B., Goroshin, R., Rabinowitz, N., Pascanu, R., Beattie, C., Petersen, S., Sadik, A., Gaffney, S., King, H., Kavukcuoglu, K., Hassabis, D., Hadsell, R., Kumaran, D., 2018. Vector-based navigation using grid-like representations in artificial agents. Nature 557, 429–433.
Bankes, S.C., 2002. Agent-based modeling: a revolution? Proc. Natl. Acad. Sci. 99, 7199–7200.
Batty, M., 2013. The New Science of Cities. MIT Press, Cambridge, MA.
Batty, M., 2008. Fifty years of urban modeling: macro-statics to micro-dynamics, in: Albeverio, S., Andrey, D., Giordano, P., Vancheri, A. (Eds.), The Dynamics of

Complex Urban Systems: An Interdisciplinary Approach. Physica-Verlag Heidelberg, Mendrisio, Switzerland, pp. 1–20.
Batty, M., 1976. Urban Modelling: Algorithms, Calibrations, Predictions. Cambridge University Press, Cambridge, MA.
Bonabeau, E., 2002. Agent-based modeling: methods and techniques for simulating human systems. Proc. Natl. Acad. Sci. 99, 7280–7287.
Borrill, P.L., Tesfatsion, L., 2011. Agent-based modeling: the right mathematics for the social sciences? In: Davis, J.B., Hands, D.W. (Eds.), The Elgar Companion to Recent Economic Methodology. Edward Elgar Publishing, Northampton, MA, pp. 228–258.
Brantingham, P.L., Glasser, U., Kinney, B., Singh, K., Vajihollahi, M., 2005. A computational model for simulating spatial aspects of crime in urban environments. 2005 IEEE Int. Conf. Syst. Man Cybern. 4, 3667–3674.
Brown, D.G., Robinson, D.T., An, L., Nassauer, J.I., Zellner, M., Rand, W., Riolo, R., Page, S.E., Low, B., Wang, Z., 2008. Exurbia from the bottom-up: confronting empirical challenges to characterizing a complex system. Geoforum 39, 805–818.
Cardinot, M., O'Riordan, C., Griffith, J., Perc, M., 2019. Evoplex: a platform for agent-based modeling on networks. SoftwareX 9, 199–204. https://doi.org/10.1016/j.softx.2019.02.009.
Cheney, D.L., Seyfarth, R.M., 1992. How Monkeys See the World: Inside the Mind of Another Species. University of Chicago Press, Chicago, IL.
Chimmula, V.K.R., Zhang, L., 2020. Time series forecasting of COVID-19 transmission in Canada using LSTM networks. Chaos Solitons Fractals 135. https://doi.org/10.1016/j.chaos.2020.109864.
Clay, R., Kieu, L.-M., Ward, J.A., Heppenstall, A., Malleson, N., 2020. Towards real-time crowd simulation under uncertainty using an agent-based model and an unscented Kalman filter. In: Demazeau, Y., Holvoet, T., Corchado, J.M., Costantini, S. (Eds.), Advances in Practical Applications of Agents, Multi-Agent Systems, and Trustworthiness. The PAAMS Collection. Springer International Publishing, Cham, pp. 68–79.
Coleman, J.S., 1987. Microfoundations and macrosocial behavior. In: Alexander, J.C., Giesen, B., Munch, R., Smelser, N.J. (Eds.), The Micro-Macro Link. University of California Press, Berkeley, CA, pp. 153–173.
Conte, R., Paolucci, M., 2014. On agent-based modeling and computational social science. Front. Psychol. 10.3389/fpsyg.2014.00668.
Couclelis, H., 2002. Why I no longer work with agents: a challenge for abms of human-environment interactions. In: Parker, D.C., Berger, T., Manson, S.M. (Eds.), Meeting the Challenge of Complexity. Presented at the Special Workshop On Land-Use/Land-Cover Change (October 4–7, 2001). Center for Spatially Integrated Social Science University of California at Santa Barbara, Irvine, California, pp. 14–16.
Crabtree, S.A., Bocinsky, R.K., Hooper, P.L., Ryan, S.C., Kohler, T.A., 2017. How to make a polity (in the central Mesa Verde region). Am. Antiq. 82, 71–95.
Cranmer, M., Sanchez-Gonzalez, A., Battaglia, P., Xu, R., Cranmer, K., Spergel, D., Ho, S., 2020. Discovering Symbolic Models from Deep Learning With Inductive Biases. ArXiv200611287 CsLG.
Crawford, T.W., Messina, J.P., Manson, S.M., O'Sullivan, D., 2005. Complexity science, complex systems, and land-use research. Environ. Plan. B Plan. Des. 32, 792–798.
Crols, T., Malleson, N., 2019. Quantifying the ambient population using hourly population footfall data and an agent-based model of daily mobility. Geoinformatica 23, 201–220. https://doi.org/10.1007/s10707-019-00346-1.
Crooks, A.T., 2010. Constructing and implementing an agent-based model of residential segregation through vector GIS. Int. J. Geogr. Inf. Sci. 24, 661–675.
Crooks, A.T., Hailegiorgis, A.B., 2014. An agent-based modeling approach applied to the spread of cholera. Environ. Model. Softw. 62, 164–177.
Crooks, A.T., Wise, S., 2013. GIS and agent-based models for humanitarian assistance. Comput. Environ. Urban Syst. 41, 100–111. https://doi.org/10.1016/j.compenvurbsys.2013.05.003.
Cumming, G.S., 2008. Complexity Theory for a Sustainable Future. Columbia Univ. Press, New York, NY.
DeAngelis, D.L., Diaz, S.G., 2019. Decision-making in agent-based modeling: a current review and future prospectus. Front. Ecol. Evol. 6, 237. https://doi.org/10.3389/fevo.2018.00237.
DeAngelis, D.L., Gross, L.J., 1992. Individual-Based Models and Approaches in Ecology: Populations, Communities and Ecosystems. Chapman and Hall, New York, NY.
Ding, Y., Densham, P.J., 1996. Spatial strategies for parallel spatial modelling. Int. J. Geogr. Inf. Syst. 10, 669–698. https://doi.org/10.1080/02693799608902104.
Eliassen, S., Andersen, B.S., Jørgensen, C., Giske, J., 2016. From sensing to emergent adaptations: modelling the proximate architecture for decision-making. Ecol. Model., Next generation ecological model., concepts, and theory: struct. realism, emergence, and predictions 326, 90–100. https://doi.org/10.1016/j.ecolmodel.2015.09.001.
Eliassen, S., Jørgensen, C., Mangel, M., Giske, J., Whitlock, A.E., E.M.C., 2009. Quantifying the adaptive value of learning in foraging behavior. Am. Nat. 174, 478–489. https://doi.org/10.1086/605370.
Evans, M.R., Grimm, V., Johst, K., Knuuttila, T., Langhe de, R., Lessells, C.M., Merz, M., O'Malley, M.A., Orzack, S.H., Weisberg, M., Wilkinson, D.J., Wolkenhauer, O., Benton, T.G., 2013. Do simple models lead to generality in ecology? Trends Ecol. Evol. 28, 578–583. https://doi.org/10.1016/j.tree.2013.05.022.
Fan, W., Ma, Y., Li, Q., He, Y., Zhao, E., Tang, J., Yin, D., 2019. Graph neural networks for social recommendation. World Wide Web Conf. 417–426. 10.1145/3308558.3313488.
Folke, C., Carpenter, S.R., Walker, B., Scheffer, M., Chapin, T., Rockström, J., 2010. Resilience thinking: integrating resilience, adaptability and transformability. Ecol. Soc. 15, 20.
Ghorbani, A., Dijkema, G., Schrauwen, N., 2015. Structuring qualitative data for agent-based modelling. J. Artif. Soc. Soc. Simul. 18, 2.
Gimblett, H.R., 2002. Integrating Geographic Information Systems and Agent-Based Modeling Techniques for Simulating Social and Ecological Processes. Oxford University Press, Oxford, GB; New York, NY, USA.
Giske, J., Eliassen, S., Fiksen, Ø., Jakobsen, P.J., Aksnes, D.L., Jørgensen, C., Mangel, M., Associate Editor: Russell Bonduriansky, Editor: Troy Day, 2013. Effects of the emotion system on adaptive behavior. Am. Nat. 182, 689–703. https://doi.org/10.1086/673533.
Giske, J., Eliassen, S., Fiksen, Ø., Jakobsen, P.J., Aksnes, D.L., Mangel, M., Jørgensen, C., 2014. The emotion system promotes diversity and evolvability. Proc R Soc B 281, 20141096. https://doi.org/10.1098/rspb.2014.1096.
Gong, Z., Tang, W., Bennett, D.A., Thill, J.-C., 2013. Parallel agent-based simulation of individual-level spatial interactions within a multicore computing environment. Int. J. Geogr. Inf. Sci. 27, 1152–1170. https://doi.org/10.1080/13658816.2012.741240.
Grimm, V., 1999. Ten years of individual-based modelling in ecology: what have we learned and what could we learn in the future? Ecol. Model. 115, 129–148.
Grimm, V., Augusiak, J., Focks, A., Frank, B.M., Gabsi, F., Johnston, A.S.A., Liu, C., Martin, B.T., Meli, M., Radchuk, V., Thorbek, P., Railsback, S.F., 2014. Towards better modelling and decision support: documenting model development, testing, and analysis using TRACE. Ecol. Model. 280, 129–139.
Grimm, V., Berger, U., 2016. Robustness analysis: deconstructing computational models for ecological theory and applications. Ecol. Model. 326, 162–167.
Grimm, V., Berger, U., Bastiansen, F., Eliassen, S., Ginot, V., Giske, J., Goss-Custard, J., Grand, T., Heinz, S.K., Huse, G., Huth, A., Jepsen, J.U., Jørgensen, C., Mooij, W.M., Müllera, B., Pe'er, G., Piou, C., Railsback, S.F., Robbins, A.M., Robbins, M.M., Rossmanith, E., Rüger, N., Strand, E., Souissi, S., Stillman, R.A., Vabø, R., Visser, U., DeAngelis, D.L., 2006. A standard protocol for describing individual-based and agent-based models. Ecol. Model. 198, 115–126.
Grimm, V., Berger, U., DeAngelis, D.L., Polhill, J.G., Giske, J., Railsback, S.F., 2010. The ODD protocol: a review and first update. Ecol. Model. 221, 2760–2768.
Grimm, V., Johnston, A.S.A., Thulke, H.-H., Forbes, V.E., Thorbek, P., 2020a. Three questions to ask before using model outputs for decision support. Nat. Commun. 11, 4959. https://doi.org/10.1038/s41467-020-17785-2.
Grimm, V., Railsback, S.F., 2012a. Designing, formulating, and communicating agent-based models. In: Heppenstall, A.J., Crooks, A.T., See, L.M., Batty, M. (Eds.), Agent-Based Models of Geographical Systems. Springer, New York, NY, pp. 361–377.
Grimm, V., Railsback, S.F., 2012b. Pattern-oriented modelling: a 'multi-scope' for predictive systems ecology. Philos. Trans. R. Soc. B Biol. Sci. 367, 298–310.
Grimm, V., Railsback, S.F., 2005. Individual-based Modeling and Ecology. Princeton University Press, Princeton, NJ.
Grimm, V., Railsback, S.F., Vincenot, C., Berger, U., Gallagher, C., DeAngelis, D., Edmonds, B., Ge, J., Giske, J., Groeneveld, J., Johnston, A.S.A., Miles, A., Nabe-Nielson, J., Polhill, J.G., Radchuk, V., Rohwader, M.-S., Stillman, R.A., Theile, J., Ayllon, D., 2020b. The ODD protocol for describing agent-based and other simulation models: a second update to improve clarity, replication, and structural realism. J. Artif. Soc. Soc. Simul. 23 https://doi.org/10.18564/jasss.4259.
Grimm, V., Revilla, E., Berger, U., Jeltsch, F., Mooij, W.M., Railsback, S.F., Thulke, H.-H., Weiner, J., Wiegand, T., DeAngelis, D.L., 2005. Pattern-oriented modeling of agent-based complex systems: lessons from ecology. Science 310, 987–991.
Groeneveld, J.J., Müller, B., Buchmann, C.M., Dressler, G., Guo, C., Hase, N., Hoffmann, F., John, F., Klassert, C.J., Lauf, T., Liebelt, V., Nolzen, H., Pannicke, N., Schulze, J., Weise, H., Schwarz, N., 2017. Theoretical foundations of human decision-making in agent-based land use models – A review. Environ. Model. Softw. 87, 39–48.
Hassan, S., Antunes, L., Pavon, J., Gilbert, N., 2008. Stepping on earth: a roadmap for data-driven agent-based modelling, in: European Social Simulation Association Annual Conference. Brescia, Italy.
Heckbert, S., Baynes, T., Reeson, A., 2010. Agent-based modeling in ecological economics. Ann. N. Y. Acad. Sci. 1185, 39–53.
Helbing, D., Brockmann, D., Chadefaux, T., Donnay, K., Blanke, U., Woolley-Meza, O., Moussaid, M., Johansson, A., Krause, J., Schutte, S., Perc, M., 2015. Saving human lives: what complexity science and information systems can contribute. J. Stat. Phys. 158, 735–781. https://doi.org/10.1007/s10955-014-1024-9.
Heppenstall, A., Malleson, N., Crooks, A., 2016. Space, the final frontier": how good are agent-based models at simulating individuals and space in cities? Systems 4, 9.
Holovatch, Y., Kenna, R., Thurner, S., 2017. Complex systems: physics beyond physics. Eur. J. Phys. 38, 023002 https://doi.org/10.1088/1361-6404/aa5a87.
Huston, M., DeAngelis, D., Post, W., 1988. New computer models unify ecological theory. Bioscience 38, 682–691.
Irwin, E.G., Geoghegan, J., 2001. Theory, data, methods: developing spatially explicit economic models of land use change. Agric. Ecosyst. Environ. 85, 7–24.
Karimi, M., Wu, D., Wang, Z., Shen, Y., 2019. Explainable Deep Relational Networks For Predicting Compound-Protein Affinities and Contacts, in: ArXiv Preprint ArXiv:1912.12553.
Karr, J.R., Sanghvi, J.C., Macklin, D.N., Gutschow, M.V., Jacobs, J.M., Jr. Bolival, B., Assad-Garcia, N., Glass, J.I., Covert, M.W., 2012. A whole-cell computational model predicts phenotype from genotype. CellCell 150, 389–401. https://doi.org/10.1016/j.cell.2012.05.044.
Kennedy, W.G., 2012. Modelling human behaviour in agent-based models. In: Heppenstall, A.J., Crooks, A.T., See, L.M., Batty, M. (Eds.), Agent-Based Models of Geographical Systems. Springer, New York, NY, pp. 167–179.
Kipf, T.N., Welling, M., 2016. Semi-supervised Classification With Graph Convolutional Networks. ArXiv160902907 CsLG.
Klemmer, K., Koshiyama, A., Flennerhag, S., 2019. Augmenting Correlation Structures in Spatial Data Using Deep Generative Models, in: ArXiv Preprint ArXiv:1905.09796.
Kravari, K., Bassiliades, N., 2015. A survey of agent platforms. J. Artif. Soc. Soc. Simul. 18, 11.

Lau, N.-C., Ploshay, J.J., 2013. Model projections of the changes in atmospheric circulation and surface climate over North America, the North Atlantic, and Europe in the twenty-first century. J. Clim. 26, 9603–9620. https://doi.org/10.1175/JCLI-D-13-00151.1.
Levin, S., Xepapadeas, T., Crépin, A.-S., Norberg, J., 2013. Social-ecological systems as complex adaptive systems: modeling and policy implications. Environ. Dev. Econ. 18, 111–132.
Levin, S., Xepapadeas, T., Crépin, A.S., Norberg, J., de Zeeuw, A., Folke, C., Hughes, T., Arrow, K., Barrett, S., Daily, G., 2012. Social-ecological systems as complex adaptive systems: modeling and policy implications. Environ. Dev. Econ. FirstView 1–22.
Levins, R., 1966. The strategy of model building in population biology. Am. Sci. 54, 421–431.
Lewars, E.G., 2011. Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics. Springer, New York, N.Y.
Ligmann-Zielinska, A., Siebers, P.O., Magliocca, N., Parker, D.C., Grimm, V., Du, J., Cenek, M., Radchuk, V., Arbab, N.N., Li, S., Berger, U., Paudel, R., Robinson, D.T., Jankowski, P., An, L., Ye, X., 2020. One size does not fit all': a roadmap of purpose-driven mixed-method pathways for sensitivity analysis of agent-based models. J. Artif. Soc. Soc. Simul. 23, 6.
Lindkvist, E., Basurto, X., Schlüter, M., 2017. Micro-level explanations for emergent patterns of self-governance arrangements in small-scale fisheries—A modeling approach. PLoS ONE 104, 107–118.
Lindkvist, E., Norberg, J., 2014. Modeling experiential learning: the challenges posed by threshold dynamics for sustainable renewable resource management. Ecol. Econ. 104, 107–118.
Liu, J., 1993. ECOLECON: a spatially-explicit model for ECOLogical-ECONomics of species conservation in complex forest landscapes. Ecol. Model. 70, 63–87.
Liu, J., Dietz, T., Carpenter, S.R., Alberti, M., Folke, C., Moran, E., Pell, A.N., Deadman, P., Kratz, T., Lubchenco, J., Ostrom, E., Ouyang, Z., Provencher, W., Redman, C.L., Schneider, S.H., Taylor, W.W., 2007. Complexity of coupled human and natural systems. Science 317, 1513–1516.
Liu, J., Hull, V., Batistella, M., DeFries, R., Dietz, T., Fu, F., Hertel, T.W., Izaurralde, R.C., Lambin, E.F., Li, S., Martinelli, L.A., McConnell, W., Moran, E.F., Naylor, R., Ouyang, Z., Polenske, K.R., Reenberg, A., Rocha, G., de, M., Simmons, C.S., Verburg, P.H., Vitousek, P.M., Zhang, F., Zhu, C., 2013. Framing sustainability in a telecoupled world. Ecol. Soc. 18, 26.
Liu, J., Moran, E., Hertel, T., Vina, A., Nichols, S., 2014. Complex Dynamics of Telecoupled Human and Natural Systems.
Long, Y., Hu, X., 2017. Spatial partition-based particle filtering for data assimilation in wildfire spread simulation. ACM Trans. Spat. Algorithms Syst. 3, 1–33. https://doi.org/10.1145/3099471.
Ma, A., Filippi, A.M., Wang, Z., Yin, Z., 2019. Hyperspectral image classification using similarity measurements-based deep recurrent neural networks. Remote Sens 11, 194. https://doi.org/10.3390/rs11020194.
Makowsky, M.D., Rubin, J., 2013. An agent-based model of centralized institutions, social network technology, and revolution. PLoS ONE 8, e80380.
Malanson, G.P., Zeng, Y., Walsh, S.J., 2006. Complexity at advancing ecotones and frontiers. Environ. Plan. A 38, 619–632.
Malleson, N., Heppenstall, A., See, L., 2010. Crime reduction through simulation: an agent-based model of burglary. Comput. Environ. Urban Syst. 34, 236–250.
Malleson, N., Heppenstall, A., See, L., Evans, A., 2013. Using an agent-based crime simulation to predict the effects of urban regeneration on individual household burglary risk. Environ. Plan. B Urban Anal. City Sci. 40, 405–426.
Malleson, N., Minors, K., Kieu, L.-.M., Ward, J.A., West, A., Heppenstall, A., 2020. Simulating crowds in real time with agent-based modelling and a particle filter. J. Artif. Soc. Soc. Simul. 23, 3. https://doi.org/10.18564/jasss.4266.
Manson, S., An, L., Clarke, K.C., Heppenstall, A., Koch, J., Krzyzanowski, B., Morgan, F., O'Sullivan, D., Runck, B.C., Shook, E., Tesfatsion, L., 2020. Methodological issues of spatial agent-based models. J. Artif. Soc. Soc. Simul. 23, 3. https://doi.org/10.18564/jasss.4174.
Manson, S.M., 2002. Calibration, verification, and validation. In: Parker, D.C., Berger, T., Manson, S.M. (Eds.), Meeting the Challenge of Complexity. Presented at the Special Workshop On Land-Use/Land-Cover Change (October 4–7, 2001). Center for Spatially Integrated Social Science University of California at Santa Barbara, Irvine, California, pp. 42–47.
Manson, S.M., 2001. Simplifying complexity: a review of complexity theory. Geoforum 32, 405–414.
Martin, B.T., Jager, T., Nisbet, R.M., Preuss, T.G., Grimm, V., 2013. Predicting population dynamics from the properties of individuals: a cross-level test of dynamic energy budget theory. Am. Nat. 181, 506–519.
Milner-Gulland, E.J., 2012. Interactions between human behaviour and ecological systems. Philos. Trans. R. Soc. B Biol. Sci. 367, 270–278.
Müller, B., Bohn, F., Dreßler, G., Groeneveld, J., Klassert, C., Martin, R., Schlüter, M., Schulze, J., Weise, H., Schwarz, N., 2013. Describing human decisions in agent-based models–ODD+ D, an extension of the ODD protocol. Environ. Model. Softw. 48, 37–48.
Murphy, J.M., Sexton, D.M.H., Barnett, D.N., Jones, G.S., Webb, M.J., Collins, M., Stainforth, D.A., 2004. Quantification of modelling uncertainties in a large ensemble of climate change simulations. Nature 430, 768–772.
National Research Council, 2014. Advancing Land Change Modeling: Opportunities and Research Requirements. The National Academies Press, Washington, DC.
Ostrom, E., 2009. A general framework for analyzing sustainability of social-ecological systems. Science 325, 419–422.
O'Sullivan, D., Manson, S.M., 2015. Do physicists have geography envy? and what can geographers learn from it? Ann. Assoc. Am. Geogr. 105, 704–722.
O'Sullivan, D., Millington, J., Perry, G., Wainwright, J., 2012. Agent-based models–because they're worth it? In: Heppenstall, A.J., Crooks, A.T., See, L.M., Batty, M. (Eds.), Agent-Based Models of Geographical Systems. Springer, New York, NY, pp. 109–124.
Othman, N.B., Legara, E.F., Selvam, V., Monterola, C., 2015. A data-driven agent-based model of congestion and scaling dynamics of rapid transit systems. J. Comput. Sci. 10, 338–350.
Parker, D.C., Manson, S.M., Janssen, M.A., Hoffmann, M.J., Deadman, P., 2003. Multi-agent systems for the simulation of land-use and land-cover change: a review. Ann. Assoc. Am. Geogr. 93, 314–337.
Perc, M., 2017. Stability of subsystem solutions in agent-based models. Eur. J. Phys. 39, 014001 https://doi.org/10.1088/1361-6404/aa903d.
Polasky, S., Zeeuw, A., Wagener, F., 2011. Optimal management with potential regime shifts. J. Environ. Econ. Manag. 62, 229–240.
Polhill, J.G., 2010. ODD updated. J. Artif. Soc. Soc. Simul. 13, 9.
Polhill, J.G., Parker, D., Brown, D., Grimm, V., 2008. Using the ODD protocol for describing three agent-based social simulation models of land-use change. J. Artif. Soc. Soc. Simul. 11, 3.
Poteete, A.R., Janssen, M.A., Ostrom, E., 2010. Working Together: Collective Action, the Commons, and Multiple Methods in Practice. Princeton University Press, Princeton, NJ.
Pumain, D., Sanders, L., 2013. Theoretical principles in interurban simulation models: a comparison. Environ. Plan. Econ. Space 45, 2243–2260.
Rai, S., Hu, X., 2013. Behavior pattern detection for data assimilation in agent-based simulation of smart environments. 2013 IEEEWICACM Int. Jt. Conf. Web Intell. WI Intell. Agent Technol. IAT 2, 171–178.
Railsback, S., Ayllón, D., Berger, U., Grimm, V., Lytinen, S., Sheppard, C., Thiele, J., 2017. Improving execution speed of models implemented in NetLogo. J. Artif. Soc. Soc. Simul. 20, 3.
Railsback, S., Lytinen, S., Jackson, S., 2006. Agent-based simulation platforms: review and development recommendations. Simulation 82, 609–623. https://doi.org/10.1177/0037549706073695.
Railsback, S.F., Grimm, V., 2019. Agent-Based and Individual-Based Modeling: A Practical Introduction, 2nd ed. Princeton University Press, Princeton, New Jersey.
Railsback, S.F., Grimm, V., 2012. Agent-Based and Individual-Based Modeling: A Practical Introduction. Princeton University Press, Princeton, New Jersey.
Railsback, S.F., Harvey, B.C., 2013. Trait-mediated trophic interactions: is foraging theory keeping up? Trends Ecol. Evol. 28, 119–125.
Railsback, S.F., Harvey, B.C., 2002. Analysis of habitat-selection rules using an individual-based model. Ecology 83, 1817–1830.
Ramanath, A.M., Gilbert, N., 2004. The design of participatory agent-based social simulations. J. Artif. Soc. Soc. Simul. 7.
Rao, A.S., Georgeff, M.P., 1991. Modeling rational agents within a BDI-architecture. In: Allen, J., Fikes, R., Sandewall, E. (Eds.), Principles of Knowledge Representation and Reasoning: Proceedings of the Second International Conference. Morgan Kaufmann Publishers, Inc., San Mateo, CA, pp. 473–484.
Rindfuss, R.R., Entwisle, B., Walsh, S.J., An, L., Badenoch, N., Brown, D.G., Deadman, P., Evans, T.P., Fox, J., Geoghegan, J., Gutmann, M., Kelly, M., Linderman, M., Liu, J., Malanson, G.P., Mena, C.F., Messina, J.P., Moran, E.F., Parker, D.C., Parton, W., Prasartkul, P., Robinson, D.T., Sawangdee, Y., Vanwey, L.K., Verburg, P.H., 2008. Land use change: complexity and comparisons. J. Land Use Sci. 3, 1–11.
Robinson, D.T., Brown, D.G., Parker, D.C., Schreinemachers, P., Janssen, M.A., Huigen, M., Wittmer, H., Gotts, N., Promburom, P., Irwin, E., Berger, T., Gatzweiler, F., Barnaud, C., 2007. Comparison of empirical methods for building agent-based models in land use science. J. Land Use Sci. 2, 31–55.
Roughgarden, J., 2012. Individual based models in ecology: an evaluation, or how not to ruin a good thing. Presented At the Philosophy of Science Association Biennial Meeting, San Diego, CA.
Scheiter, S., Langan, L., Higgins, S.I., 2013. Next-generation dynamic global vegetation models: learning from community ecology. New Phytol 198, 957–969.
Schill, C., Anderies, J.M., Lindahl, T., Folke, C., Polasky, S., Cárdenas, J.C., Crépin, A.-.S., Janssen, M.A., Norberg, J., Schlüter, M., 2019. A more dynamic understanding of human behaviour for the Anthropocene. Nat. Sustain. 2, 1075–1082. https://doi.org/10.1038/s41893-019-0419-7.
Schlüter, M., Baeza, A., Dressler, G., Frank, K., Groeneveld, J., Jager, W., Janssen, M.A., McAllister, R.R.J., Müller, B., Orach, K., Schwarz, N., Wijermans, N., 2017. A framework for mapping and comparing behavioural theories in models of social-ecological systems. Ecol. Econ. 131, 21–35.
Schlüter, M., Mcallister, R.R.J., Arlinghaus, R., Bunnefeld, N., Eisenack, K., Hoelker, F., Milner-Gulland, E.J., Mueller, B., 2012a. New horizons for managing the environment: a review of coupled social-ecological systems modeling. Nat. Resour. Model. 25, 219–272. https://doi.org/10.1111/j.1939-7445.2011.00108.x.
Schlüter, M., Mcallister, R.R.J., Arlinghaus, R., Bunnefeld, N., Eisenack, K., Holker, F., Milner-Gulland, E.j., Muller, B., Nicholson, E., Quaas, M., Stoven, M., 2012b. New horizons for managing the environment: a review of coupled social-ecological systems modeling. Nat. Resour. Model. 25, 219–272. https://doi.org/10.1111/j.1939-7445.2011.00108.x.
Schmidt, B., 2002. The modelling of human behaviour: the PECS reference model. In: Verbraeck, A., Krug, W. (Eds.), Presented At the Proceedings 14th European Simulation Symposium. SCS Europe Bvba, Dresden, Germany.
Schmolke, A., Thorbek, P., DeAngelis, D.L., Grimm, V., 2010. Ecological models supporting environmental decision making: a strategy for the future. Trends Ecol. Evol. 25, 479–486.
Schulze, J., Müller, B., Groeneveld, J., Grimm, V., 2017. Agent-based modelling of social-ecological systems: achievements, challenges, and a way forward. J. Artif. Soc. Soc. Simul. 20, 8.

Seidl, R., 2015. A functional-dynamic reflection on participatory processes in modeling projects. Ambio 44, 750–765.
Seppelt, R., Richter, O., 2005. It was an artefact not the result": a note on systems dynamic model development tools. Environ. Model. Softw. 20, 1543–1548.
Shaw, S.-L., Tsou, M.-H., Ye, X., 2016. Human dynamics in the mobile and big data era. Int. J. Geogr. Inf. Sci. 30, 1687–1693.
Shook, E., Wang, S., Tang, W., 2013. A communication-aware framework for parallel spatially explicit agent-based models. Int. J. Geogr. Inf. Sci. 27, 2160–2181. https://doi.org/10.1080/13658816.2013.771740.
Sinsabaugh, R.L., Manzoni, S., Moorhead, D.L., Richter, A., 2013. Carbon use efficiency of microbial communities: stoichiometry, methodology and modelling. Ecol. Lett. 16, 930–939.
Stillman, R.A., Railsback, S.F., Giske, J., Berger, U., Grimm, V., 2015. Making predictions in a changing world: the benefits of individual- based ecology. Bioscience 65, 140–145.
Swarup, S., Mortveit, H.S., 2020. Live Simulations, in: Proceedings of the 19th International Conference On Autonomous Agents and MultiAgent Systems, AAMAS '20. International Foundation For Autonomous Agents and Multiagent Systems, Richland, SC, pp. 1721–1725.
Tang, W., Bennett, D.A., 2011. Parallel agent-based modeling of spatial opinion diffusion accelerated using graphics processing units. Ecol. Model. 222, 3605–3615.
Tang, W., Bennett, D.A., 2010. The explicit representation of context in agent-based models of complex adaptive spatial systems. Ann. Assoc. Am. Geogr. 100, 1128–1155.
Tang, W., Bennett, D.A., Wang, S., 2011. A parallel agent-based model of land use opinions. J. Land Use Sci. 6, 121–135.
Tang, W., Jia, M., 2014. Global sensitivity analysis of a large agent-based model of spatial opinion exchange: a heterogeneous multi-GPU acceleration approach. Ann. Assoc. Am. Geogr. 104, 485–509. https://doi.org/10.1080/00045608.2014.892342.
Tang, W., Wang, S., 2009. HPABM: a hierarchical parallel simulation framework for spatially-explicit agent-based models. Trans. GIS 13, 315–333.
Tesfatsion, L., 2017. Modeling economic systems as locally-constructive sequential games. J. Econ. Methodol. 24, 384–409.
Thiele, J.C., Grimm, V., 2015. Replicating and breaking models: good for you and good for ecology. Oikos 124, 691–696.
Tubaro, P., Casilli, A.A., 2010. An ethnographic seduction": how qualitative research and agent-based models can benefit each other. Bull. Sociol. Methodol. 106, 59–74.
Turner II, B.L., Matson, P.A., McCarthy, J.J., Corell, R.W., Christensen, L., Eckley, N., Hovelsrud-Broda, G.K., Kasperson, J.X., Kasperson, R.E., Luers, A., Martello, M.L., Mathiesen, S., Naylor, R., Polsky, C., Pulsipher, A., Schiller, A., Selin, H., Tyler, N., 2003. Illustrating the coupled human–environment system for vulnerability analysis: three case studies. Proc. Natl. Acad. Sci. 100, 8080–8085.
Verburg, P.H., Dearing, J.A., Dyke, J.G., Leeuw van der, S., Seitzinger, S., Steffen, W., Syvitski, J., 2016. Methods and approaches to modelling the anthropocene. Glob. Environ. Change 39, 328–340. https://doi.org/10.1016/j.gloenvcha.2015.08.007.
VidalMata, R.G., Banerjee, S., RichardWebster, B., Albright, M., Davalos, P., McCloskey, S., Miller, B., Tambo, A., Ghosh, S., Nagesh, S., Yuan, Y., Hu, Y., Wu, J., Yang, W., Zhang, X., Liu, J., Wang, Z., Chen, H.-T., Huang, T.-W., Chin, W.-C., Li, Y.-C., Lababidi, M., Otto, C., Scheirer, W.J., 2020. Bridging the gap between computational photography and visual recognition. IEEE Trans. Pattern Anal. Mach. Intell. 10.1109/TPAMI.2020.2996538.
Vincenot, C.E., 2018. How new concepts become universal scientific approaches: insights from citation network analysis of agent-based complex systems science. Proc. R. Soc. B Biol. Sci. 28, 20172360.
Vincenot, C.E., Giannino, F., Rietkerk, M., Moriya, K., Mazzoleni, S., 2011. Theoretical considerations on the combined use of system dynamics and individual-based modeling in ecology. Ecol. Model. 222, 210–218.
Vincenot, C.E., Mazzoleni, S., Parrott, L., 2016. Hybrid solutions for the modeling of complex environmental systems. Front. Environ. Sci. 4, 53.
Voinov, A., Bousquet, F., 2010. Modelling with stakeholders. Environ. Model. Softw. 25, 1268–1281.
Wang, S., Anselin, L., Bhaduri, B., Crosby, C., Goodchild, M.F., Liu, Y., Nyerges, T.L., 2013. CyberGIS software: a synthetic review and integration roadmap. Int. J. Geogr. Inf. Sci. 27, 2122–2145.
Wang, S., Armstrong, M.P., 2003. A quadtree approach to domain decomposition for spatial interpolation in Grid computing environments. Parallel Comput. 29, 1481–1504. https://doi.org/10.1016/j.parco.2003.04.003.
Wang, X., He, X., Wang, M., Feng, F., Chua, T.-.S., 2019. Neural graph collaborative filtering. SIGIR19 Proc. 42nd Int. ACM SIGIR Conf. Res. Dev. Inf. Retr. 165–174. 10.1145/3331184.3331267.
Ward, J.A., Evans, A.J., Malleson, N.S., 2016. Dynamic calibration of agent-based models using data assimilation. R. Soc. Open Sci.
Wilensky, U., 1999. NetLogo. Center For Connected Learning and Computer-Based Modeling(CCL). Northwestern University., Evanston, IL.
Wilensky, U., Rand, W., 2015. An Introduction to Agent-Based modeling: Modeling natural, social, and Engineered Complex Systems With NetLogo. MIT Press, Cambridge, MA.
Wilkinson, B., Allen, M., 2004. Parallel Programming: Techniques and Applications Using Networked Workstations and Parallel Computers, 2nd ed. Prentice Hall, Upper Saddle River, NJ.
Will, M., Groeneveld, J., Frank, K., Müller, B., 2020. Combining social network analysis and agent-based modelling to explore dynamics of human interaction: a review. Socio - Environ. Syst. Model. Open - Access Sch. J. 2 https://doi.org/10.18174/sesmo.2020a16325.
Wilson, E.O., 1975. Sociobiology. Harvard University Press, Cambridge, MA.
Yang, L., Gilbert, N., 2008. Getting away from numbers: using qualitative observation for agent-based modeling. Adv. Complex Syst. 11, 175–185.
Ye, X., He, C., 2016. The new data landscape for regional and urban analysis. GeoJournal 81, 811–815. https://doi.org/10.1007/s10708-016-9737-8.
Ye, X., Lee, J., 2016. Integrating geographic activity space and social network space to promote healthy lifestyles. SIGSPATIAL Spec 8, 20–33.
Ying, Z., You, J., Morris, C., Ren, X., Hamilton, W., Leskovec, J., 2018. Hierarchical graph representation learning with differentiable pooling. Adv. Neural Inf. Process. Syst. 31, 4800–4810.
Zhang, H., Vorobeychik, Y., Letchford, J., Lakkaraju, K., 2016. Data-driven agent-based modeling, with application to rooftop solar adoption. Auton. Agents Multi-Agent Syst. 30, 1023–1049. https://doi.org/10.1007/s10458-016-9326-8.
Zhang, M., Chen, Y., 2018. Link prediction based on graph neural networks, in: Advances in Neural Information Processing Systems 31 (NIPS 2018). pp. 5165–5175.
Zhu, D., Liu, Y., 2018. Modelling spatial patterns using graph convolutional networks (short paper). In: Winter, S., Griffin, A., Sester, M. (Eds.), 10th International Conference on Geographic Information Science (GIScience 2018), Leibniz International Proceedings in Informatics (LIPIcs). Schloss Dagstuhl–Leibniz-Zentrum fuer Informatik, Dagstuhl, Germany, p. 73:1–73:7.
Zvoleff, A., An, L., 2014. Analyzing human-landscape interactions: tools that integrate. Environ. Manage., Special issue on "The Future of Human-Landscape Interact: Drawing on the Past, Anticipating the Future" 104, 723–745.