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Review Article

Complex adaptive systems science in the era of global sustainability crisis

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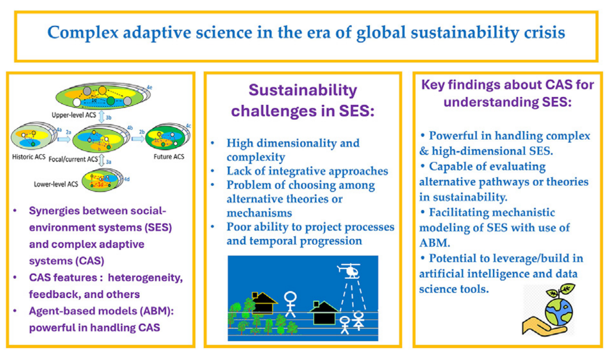
HIGHLIGHTS

- Social-environmental systems (SES) are complex adaptive systems (CAS).
- CAS handles the high dimensionality and complexity challenges in SES.
- CAS helps evaluate alternative pathways or theories in sustainability.
- Agent-based models help mechanistic modeling of SES with sustainability challenges.
- Agents' behaviors can be better derived by artificial intelligence and data science tools.

GRAPHICAL ABSTRACT



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ABSTRACT

A significant number and range of challenges besetting sustainability can be traced to the actions and interactions of multiple autonomous agents (people mostly) and the entities they create (e.g., institutions, policies, social network) in the corresponding social-environmental systems (SES). To address these challenges, we need to understand decisions made and actions taken by agents, the outcomes of their actions, including the feedbacks on the corresponding agents and environment. The science of complex adaptive systems—complex adaptive systems (CAS) science—has a significant potential to handle such challenges. We address the advantages of CAS science for sustainability by identifying the key elements and challenges in sustainability science, the generic features of CAS, and the key advances and challenges in modeling CAS. Artificial intelligence and data science combined with agent-based modeling promise to improve understanding of agents' behaviors, detect SES structures, and formulate SES mechanisms.

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1. Introduction

The Anthropocene witnesses unprecedented conditions and challenges about human-environment relationships (Steffen et al., 2015; Turner, 2022). These conditions are created by the escalating demands placed on the global environment by the largest population with the highest level of material consumption in the history of humankind. They generate challenges that range from equitable consumption (Costanza et al., 2014; United Nations, 2016) to the consequences of consumption on the functioning of the Earth system (Lade et al., 2020). Together, these challenges have emboldened the search for sustainability—meeting the material needs of the humankind more equitably and for future generations, while not threatening the capacity of Earth system functioning and delivering the ecosystem services (Board on Sustainable Development, National Research Council, 1999; Kates et al., 2001; The World Commission on Environment and Development, 1987). This search, in turn, has given rise to sustainability science, a use-inspired research field seeking to advance understanding about critical elements that promote sustainable development (Bettencourt and Kaur, 2011; Clark and Harley, 2020; Kates, 2011). It constitutes "a new social contract for science" (Lubchenco, 1998), akin to agricultural or medical research (Kates, 2011), in which the approach to problem solving remains within the explanatory structure and methods of science but maintains a normative element—the goal of sustainability (Clark and Harley, 2020).

Human-environment interactions reside at the core of the sustainability science, and are addressed as social-environmental systems (SESs: aka social-ecological systems, coupled human and natural systems, or nature–society systems (Liu et al., 2007a, 2007b; Schlüter et al., 2023a)), which behave as complex adaptive systems (CAS) (Preiser et al., 2018; Section 3) in many, if not most, instances. Comprehensive synthesis articles (Bettencourt and Kaur, 2011; Clark and Harley, 2020; Kates, 2011; Liu et al., 2015, 2018) and online repertoires (Harley and Clark, 2020; SDSN Association 2019) indicate that SES maintain at least three overarching elements: actors, environment, and outcome (detail in Supplemental file A) (Kates, 2011). These three elements correspond to agents, environment, and emergence in CAS, although these elements are more restrictive than those to which CAS at large has addressed (detail in Supplemental file B). In SES science agents/actors must be people-based (i.e., from individuals to states), environment must include biophysical and built systems, and the outcome need not be emergent. Understanding the interactions in question and their outcomes could be enhanced for many of the problems addressed in sustainability science by improved engagement with the concepts of CAS and its tools and methods: agent-based modeling (ABM), artificial intelligence (AI), and data science.

This article is structured as follows. The theoretical background, Section 2, is comprised of three parts. Section 2.1 identifies four major challenges in sustainability science, namely *high dimensionality/complexity, the need for systems integration, choosing from alternative theories*, and *the need to have temporal progression*. CAS science and its major method, ABM, provide unique strengths to tackle these challenges. Section 2.2 demonstrates that despite substantial efforts over the last two decades, CAS/ABM is quite underrepresented as a means to address research problems in sustainability science. As such, an articulation of the synergies to be gained by more attention to the linkages in question constitutes Section 2.3. This articulation, Section 3, identifies what CAS and ABM are and why/how they can contribute to the four challenges of sustainability (Sections 3.1 through 3.4). These contributions notwithstanding, three major constraints of CAS and ABM, are identified and discussed (Section 4): difficulties in dealing with system structure and cross-scale influences, detecting causality, and using qualitative data. AI offers a means to elegantly handle these constraints. Finally, Section 5 points to future directions of CAS/ABM in sustainability science.

2. Theoretical background

2.1. Central challenges in sustainability science

Several central challenges emerge in sustainability science, pursuant to its goal of sustainable development (Clark and Harley, 2020), that are prevalent in the synthesis articles and online repertoires noted above. It is difficult, if not impossible, to present a full spectrum of theories, approaches, advances, findings, and potential development pathways pertaining to the challenges in question. Here, we focus on several broad challenges to sustainability science in which CAS (similar to agent-based complex systems as labeled by Grimm and colleagues, Grimm et al., 2005) science and ABM may provide potentials to resolve, especially in light of AI. CAS science examines "dynamic networks of many interacting agents" (Grimm et al., 2005) with an emphasis on information about entities at a lower level(s) of the system, theories about their behavior, and the emergence of system-level properties related to particular questions (Axelrod and Cohen, 1999; Holland, 1992). Such attention dates back to at least 1970s (details in Section 3.1). As the process of perceiving, synthesizing, and inferring information by machines (Nilsson, 2009), AI may substantially empower CAS science to address sustainability challenges as noted below. In particular, we highlight the usefulness of machine learning, a branch of AI, which focuses on developing, understanding, and using methods that leverage data to improve the performance on some set of tasks.

The first challenge is a need to address the high dimensionality and complexity of SES that sustainability science examines. Such systems are highly complex given the dimensions of factors and relationships comprising them (Clark and Harley, 2020; Kates, 2011; Kates et al., 2001). Following Clark and Harley (2020), the generic SES of sustainability science includes the interactions of institutions (governance), actors, and resources (biophysical world at large) regarding consumption and production goals. These elements maintain high heterogeneity at the lower (micro or local) and focal (*meso*) spatial levels, although persistent or macro-level factors, such as climate zones or political boundaries, influence the interactions. These interactions may vary over time, affected by past conditions and leading to different outcomes, some of which may be emergent patterns, especially surprises that may come from unknown factors or causal relationships (Scheffer et al., 2012). Despite this complexity, SES are, for practical reasons, often examined by focusing on specific systems at local scales, and on lower levels of system organization. This way of handling complexity tends to draw attention to place-based or context specific outcomes, from which SES-specific strategies for achieving certain sustainability goals are derived. It is understood, however, that the overall internal organization of SES is based on more general and overarching principles (Clark and Harley, 2020; Kates et al., 2001). Focusing on the lower levels and local scales limits insights into general dynamics and principles that could enhance understanding and broader strategies. Given the high dimensionality and complexity of sustainability challenges, "silo approaches" (Grimm, 2023; Liu et al., 2018) alone may solve one problem while exacerbating others, or relieve the problem in one dimension or moment but worsen it in others.

Hence, and second, there comes the need for integrative approaches. Several frameworks for this integration have been proposed or advanced within sustainability science, foremost cast for specific problem sets common to sustainability (Ostrom, 2009; Turner, et al., 2020) such as human-nature nexus and telecoupling (e.g., Kapsar et al., 2019). At the same time, sets of metrics capturing the dimensionalities involved have been proposed, such as inclusive wealth—the "… aggregate value of all capital assets [including ecosystem services], where the value of a unit of a capital asset is measured by the contribution it makes to increasing current and future human well-being" (Polasky et al., 2015, p. 446). In one of the broadest framing, Clark and Harley (2020) propose that the spatial dynamics of human-environmental interactions at the mesoscale can act as a bridge, integrating the heterogeneity of lower-level dynamics with the more stable, macro-scale patterns and processes within the SES.

Third, choosing among alternative theories or mechanisms to explain or project human decision-making or actions is a serious challenge (An et al., 2023; Wijermans et al., 2023). For example, alternative theories of resource uses may yield highly divergent outcomes at the system level, with none outperforming the others in terms of robustness and validity (Janssen and Baggio, 2017). It is increasingly acknowledged that no single model of decision making will be able to cover all possible contexts, hence frameworks exist that help to find the most suitable decision model for a given context (Wijermans et al., 2023). Still, even for a given context, seemingly minor details of how a theory is implemented can have large effects on the system-level outcomes (Muelder and Filatova, 2018).

Fourth and last, sustainability research and applications must enable and evaluate processes and temporal progression (Clark and Harley, 2020). This temporal dimension, including depicting and predicting pathways of development affected by hysteresis and legacies effects (i.e., lag-times between cause and effect and past outcomes constraining future ones, respectively) as well as future tipping points and adaptations in human-environmental conditions (Bürgi et al., 2017), becomes a must.

2.2. Underrepresentation of CAS/ABM in sustainability science

CAS and ABM have been increasingly used to handle sustainability problems in human-environmental arenas, particularly in land use/change analysis, human-wildlife interaction, and agricultural systems (An et al., 2020a; Brown and Robinson, 2006; Müller et al., 2007; Robinson et al., 2007). We can see such popularity also from a set of review papers (An, 2012; An et al., 2021, 2023; Elsawah et al., 2020; Parker et al., 2003; Rounsevell et al., 2012; Schlüter et al., 2012). However, we believe CAS and ABM are still quite underrepresented in sustainability science literature. As pointed out in a review paper (Ioan et al., 2021), a search on the Web of Science under the key "TS=(("sustainability" OR "sustainable development") AND ("agent-based modeling" OR "agent-based simulation")) AND Language="English" returned 170 publications from January 2005 to July 2019. In comparison, a search also on the Web of Science for "sustainability" OR "sustainable development" (as topic) for 2018 alone returned 27,608 publications (also in English). Out of the above total number (170), the authors kept 87 publications that were meaningful (Ioan et al., 2021). Among the 87 publications, the top three domains were agriculture (24), transportation (13), and energy (10). This underrepresentation of CAS and ABM in sustainability science may arise from the relative unfamiliarity with CAS science and its ABM methodology (An et al., 2017, 2021).

The underrepresentation of CAS and ABM in sustainability science is also supported by our own literature search (See the endnote[1]). For example, CAS applied to addressing sustainability problems have significantly increased of late, but they comprised only about 1.24 % of all sustainability science publications as late as 2021 (Fig. 1). In addition, among the 22 generic sustainability science cases examined here, only 15 of them could benefit from using ABMs but failed to do so (Table S1 in Supplemental file C).

[1] We used a combination of (sustainability science) OR (sustainability) OR (sustainable development) for searches under "Topic" in Web of Knowledge. For the agent-based modeling related search, we use (agent-based model*) OR (agent-based model*) OR (individual-based model*) OR (individual based model*) also under Topic. The two searches are connected with an AND operator. The Queries were sent on 31 December 2021 to retrieve the entire set of papers from 2000 to December 31, 2021.

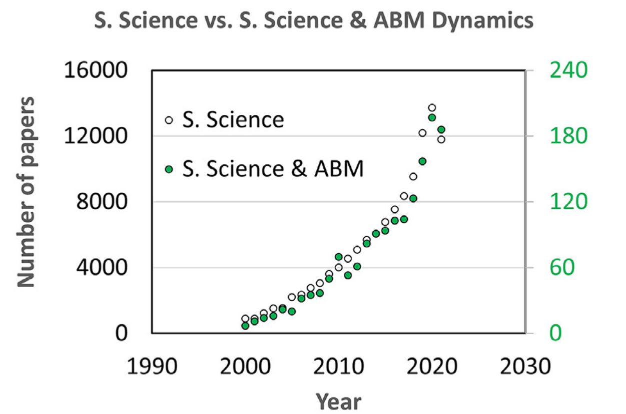

Fig. 1. Publications addressing sustainability science (# of publications under the search for the sustainability science topic; left *Y*-axis) vs. those using ABMs (# of publications under the search for both sustainability science AND ABM topic; right *Y*-axis) to address sustainability problems since 2000 (S. Science = sustainability science; for data search detail, see the endnote).

2.3. Problem statement

The literature reviewed above suggests that advances in linking CAS/ABM with sustainability science problems at large could improve understanding of sustainability problems and, perhaps, promote synergies between the two research communities. Focusing on the improvement goal, we identify the basic concepts in CAS and its major methodology of ABM, illustrate the usefulness of CAS/ABM in addressing sustainability science challenges, and point out a new opportunity arising from AI to address sustainability problems, while also advancing CAS/ABM. We envision that CAS and sustainability sciences can be integrated, with strong possibilities of leading to breakthroughs in understanding and for application of sustainability problems.

3. Contribution of CAS science to addressing sustainability challenges

3.1. Handling the high dimensionality and complexity challenges

Dating back to open systems in the mid-20th century (Von Bertalanffy, 1950) and explicit studies of complexity in the 1970s (Vemuri, 1978) and arguably in late 1940s (Weaver, 1948), CAS science has advanced to a comprehensive, complex systems framework that can address the high dimensionality and complexity problems addressed in sustainability science. Compared to Complex Systems (Holland, 1992) or Agent Societies (Conte and Paolucci, 2014) to which CAS are similar, the latter emphasizes the pivotal role of individual agents or entities (objects) that make choices, commonly to pursue a certain goal (Abar et al., 2017). Agents in CAS interact with one another (Fig. 2, dashed arrows) and the environment. Agents can possess different degrees of autonomy, proactivity, and intellectual capabilities, such as memory, knowledge, reasoning, learning, social capital, and adaptative capacity. Computationally, agents are represented as software abstractions that bundle a particular set of attributes (or traits) and methods (or actions). Algorithmically, agents follow rules ranging from very simple "if-then" (reactive decision) rules to sophisticated ones based on evaluating the future consequences of alternative decisions (Rounsevell et al., 2012). This representation builds on a unique ontology (Fig. 2) in which real-world agents are represented as heterogeneous individuals that generate the interactions in question (An, 2012; Brown and Robinson, 2006). This ontology of methodological individualism represents a shift from understanding aggregate agent features and/or relationships to the individuals and micro-level processes that constitute and explain the aggregate features (detail in Supplemental file B). At the same time, we

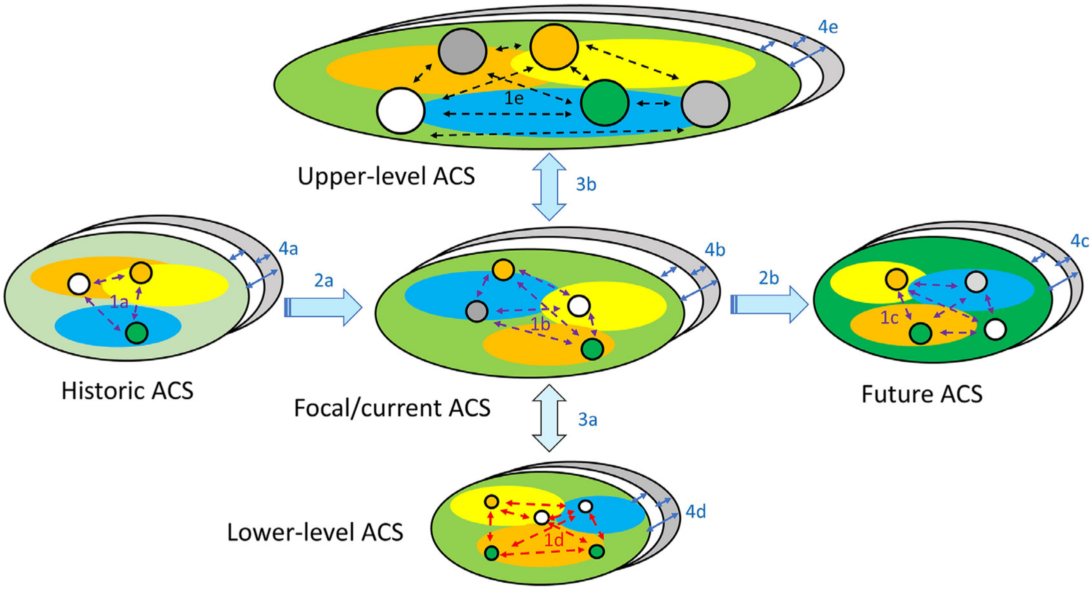

Fig. 2. Ontology of complex adaptive systems (CAS). Circles and ovals represent agents and the environment, respectively, while arrows of different colors and shapes represent heterogeneous interactions or influences between various CAS elements. The numbers and letters represent interactions among agents and those among CAS, respectively.

show that non-traditional data can help unfold dynamic patterns (detail in Supplemental file D).

Given the features in this ontology (Fig. 2), CAS science offers a comprehensive, complex systems framework applicable for the problem sets, interactions, and outcomes addressed in sustainability science. This applicability is illustrated by way of a literature survey of empirical studies in both CAS and sustainability sciences (Supplemental file C). The qualities of the CAS framework that can guide sustainability scientists and practitioners follow.

First, SES in sustainability problems can be examined in a hierarchical structure, where actors (i.e., CAS agents) at one level or location may affect and be affected by actors at other levels or locations. The sustainability literature is replete with cross-scale (lower to upper levels) interactions (detail in Supplemental file C). For example, individual migrants (lower-level actors) affect their households (focal or meso-level actors) through remittances (Dou et al., 2017; Mena et al., 2011); or wastepaper markets (upper-level actors) affect decisions of their suppliers and recyclers (focal-level actors) (Sauvageau and Frayret, 2015).[2] Also, An et al. (2020a) show that individual monkeys and monkey groups may jointly affect their movement and habitat use patterns (Supplemental file E)

Second, CAS can be employed to track the behavior of autonomous, heterogeneous, and decision-making agents that SES entertain. For instance, it can track the movement of prey and predator animals and hunters in realistic simulations, accounting for encounters, hunts, or predates on the heterogenous landscape at certain times. The resulting simulation gives rise to meaningful results when alternative behavioral models are applied to ABM, testing the reliability of various theories of social behavior of hunter–gatherers (Supplemental file F).

Third, sustainability problems commonly involve assessment of temporal dynamics. Environmental conditions at earlier times, for example, may constrain those at the current time, which may in turn further constrain those at future times. A plethora of SES case studies, for instance, examine the impacts of historic precipitation, disasters, fires, local weather conditions, and land use on the current environment (Table S2 in Supplemental file C). Similarly, adjacent or distant environments may affect and be affected by the immediate environment in question at the same level through various mechanisms, such as the telecoupling effect (Dou et al., 2020) (Table S2 in Supplemental file C). CAS has the capacity to account for these dynamics in models.

Fourth, decisions or actions of actors at one time or location may influence their own and other actors' decisions or actions, which may translate to system-level events or emerging outcomes at later times or other locations. Abundant SES examples exist regarding how agents affect one another through crop choice, land abandonment, social norm changes, coastal defensive buildings, trading of goods, and other interactions in SES (see Table S2 in Supplemental file C).

Fifth, at the system level, attention is paid to the mutual influences between SES across different levels, between parallel SES, or among different times. For instance, to project future human migrations and changes in the environment, the interactions between parallel SES in the future can be assessed by the exchange of information of migration destinations within a social network, which can be viewed as interconnection between the local system of migration origin and outside systems of migration destinations (Kniveton et al., 2011).[3]

Finally—as a result of the above points—the CAS ontology provides a framework that captures the essence of many other SES processes and dynamics, such as adaptive decision-making and the co-evolutionary aspect of SES. It guides sustainability interests in the formulation of goals, data collection, and analysis and modeling.

3.2. Providing an effective platform for systems integration

The modeling advances of CAS science point to its potential in addressing the aforementioned high dimensionality, complexity, and other problems of SES and sustainability given the following considerations:

- Agents: what agents (or actors; Supplemental file A), attributes and/or traits, and behaviors of the agents should be included at each level of the corresponding CAS or SES?
- Environment: what attributes and processes should be included (especially those affected by and feed back to affect agents) at each

[2] More examples are available in Table S2, Supplemental file C and Supplemental file E, where individual monkey and monkey group agents affect each other across focal- and upper-levels.

[3] More examples about system-level SES/CAS interactions are presented in Table S2 (under various CAS-CAS interaction subcategories).

level? In CAS, the environment can be broadly defined to be the context other than the agent under consideration, such as the space (land) and/or other agents.
- Agent-agent and agent-environment interactions: what relationships (expressed as rules, influences, or actions) among or between agents and the environment govern system dynamics at each level? What cross-level (e.g., from upper- to focal level) relationships are needed to account for systems dynamics and complexity?
- Systems-level complexity (e.g., emergence): what emerging patterns may arise from the interactions? Such patterns, often not the sum of the system's parts, cannot be analytically solved by examination of the system's parts alone.[4] This complexity includes surprises, path dependence, nonlinearity, self-organization, contingency, emergence, multifinality, and equifinality (for definitions see Liu et al. (2007a) and An (2022).

Sustainability science examines human-environment relationships in which actors/agents are people or various organizations of them and the environment is the biophysical world as modified-to-transformed by human action. It seeks to understand the interactions within and between the two subsystems. It is also open to applications of various methods and models, especially those that can handle integration among the components of SES (Turner et al., 2020). CAS science, in contrast, examines any kind of relationships, agents, and subsystem interactions (e.g., bacteria and their hosts) and has heavily leveraged the use of ABMs, although cellular automata (Taleb et al., 2004), partial differential equations (Chaplain and Anderson, 2004; Hornberg et al., 2006; Lindsay et al., 2020), cell-based stochastic modeling (Roeder and Loeffler, 2002), and structural equation modeling (Folmer et al., 2012) are not uncommon (see Table S2). Regardless of the range of agents entertained, CAS science provides a platform for systems integration applicable for sustainability science topics, including integration of data, information, and knowledge gained from case studies, stylized facts, role-playing games, and laboratory experiments (e.g., the four empirical approaches for social science research by Jansen and Ostrom (Janssen and Ostrom, 2006)). Significantly, agent-based modeling, as a prime CAS method and tool (e.g., credited to do "a new kind of science" (Wolfram, 2002)), provides a way to fuse the deductive-mechanistic and the inductive-empirical approaches that pervade different pathways toward understanding and envisioning CAS.[5]

Perhaps the most advantageous feature of ABM is its capacity to provide a platform and tool for systems integration, a major goal of sustainability science (Liu et al., 2015; Rounsevell et al., 2012). Mimicking the realistic (though tailored and simplified) structure and processes of the system under investigation (Fig. 2), ABM seeks to translate real-world actors, environment (e.g., forestland), and constraints (e.g., land use regulations; Fig. 2) into virtual agents, virtual environment (e.g., land pixels), and computerized rules (e.g., if A then B else C), offering opportunities for integrating heterogenous data, knowledge, models/methods that cross spatial, temporal, and organizational scales, disciplines, and borders (e.g., political) (An et al., 2005; Parker and Robinson, 2017) (see Supplemental file E). ABMs are powerful when modeling learning and adapting processes (An, 2012; Cumming, 2008; Milner-Gulland, 2012), accounting for heterogeneity, bounded rationality and incomplete knowledge/information, and nonlinearities (An et al., 2020b; National Research Council, 2014; Rounsevell et al., 2012), and exploring many complexity features such as path-dependence, abrupt changes, and critical thresholds, among others (An, 2022).

ABMs have been widely developed and used in CAS studies to address problems confronting social, environmental, and social-environmental systems since the 1990s (An et al., 2021; Vincenot, 2018). These endeavors have generated a rich legacy of ABM methodology, such as the Overview, Design concepts, Details (ODD) protocol and variants for model documentation (Grimm et al., 2020; Müller et al., 2013) and the Pattern-oriented Modeling (POM) approach (Grimm et al., 2005) for model validation. At the same time, ABM endeavors have enriched the literature in sustainability science in terms of modeling human behavior (An, 2012; Janssen and Baggio, 2017): for example, the frameworks for Belief-Desire-Intentions and physical, emotional, cognitive, and social factors (Conte and Paolucci, 2014; Schmidt, 2002); exploring how adaptive behavior, abrupt changes, crises or disasters, and critical transitions may generate surprising patterns in the corresponding SES (An et al., 2014; Liu et al., 2007a; National Research Council, 2014); life cycle assessment (Davis et al., 2009; Marvuglia et al., 2018); and modeling emergent macro-level outcomes and pathways under various policies or interventions (An et al., 2005; DeAngelis and Grimm, 2014; Gimblett, 2002; National Research Council, 2014).

A 2006 special issue of *Ecology and Society* (Janssen and Ostrom, 2006) constitutes a milestone in the sustainability science and ABM nexus, providing various empirical methods by which ABMs were empirically tested for SES. Aside from a variety of challenges in developing and employing ABMs such as sharp learning curve, high data demand, programming difficulties (An, 2012; An et al., 2021, 2020b; Schulze et al., 2017), the relative unfamiliarity of CAS science and ABMs in the sustainability science community (Section 2.2) highlights the timeliness and importance of this article.

3.3. Handling alternative pathways or theories in sustainability

CAS science has been wrestling with equi/multifinality (or finality) issues, which also abound in sustainability science. Equifinality—a macro-level pattern can be generated through different pathways from micro-level processes (von Bertalanffy, 1968)—makes the search for mechanistic explanations challenging. In CAS science, for instance, cooperation or betrayal in the Prisoner's Dilemma can emerge from tit-for-tat retaliation (Axelrod, 1997), strong reciprocity (Boyd et al., 2003), and group selection (Di Tosto et al., 2007), among other strategies (Conte and Paolucci, 2014). As a double-edged sword, equifinality may offer more explanatory pathways, but also question the validity of explanations because different theories can reproduce very similar or even the same macro-patterns. In contrast, multifinality—the same causes and/or starting conditions lead to very different outcomes—also poses challenges to our understanding for mechanistic approaches (An et al., 2021). For other issues related to CAS/ABM model verification and validation, we refer to An et al. (2021).

The POM approach (Grimm et al., 2005; Grimm and Railsback, 2012), overlapping with Approximate Bayesian Computing (Hartig et al., 2011) in CAS, offers a possible means to address the finality issues. It is based on the multi-criteria design, selection, and calibration of models by requiring that models can simultaneously reproduce an entire set of patterns characterizing an CAS. Often a set of broad, general patterns can more effectively reduce finality issues than trying to force a model to reproduce a single pattern, such as a time series of a single variable. Given the synergy between CAS and sustainability sciences hitherto discussed, we posit that despite the paucity of application in sustainability science, POM may prove useful to uncovering many sustainability related mechanisms, such as testing theories of certain foraging behaviors using ABM (Supplemental file F).

Given the reflexivity of human agents, the social sciences tend to approach the dynamics of the social subsystem in multiple, probabilis-

[4] In CAS science, common processes leading to emerging patterns are distilled and generalized from specific case studies or experiments, paving the way to develop, test, and refine falsifiable, generative theories that reproduce observed system dynamics (Epstein, 2014).

[5] Axelrod (1997) calls CAS type simulations a third way of doing science in contrast to inductive and deductive approaches, the two primary ways of doing science. Accounting for abductive approaches (Flach and Kakas, 2014) or plausible outcomes confined to particular observations, common in the social sciences, perhaps CAS science might be seen as a "fourth" way of doing science.

tic ways, commonly applying both quantitative and qualitative methods. Empirical models use evidence to explore outcomes and plausible, inductively derived explanations (Robinson et al., 2007). These "top-down" models reproduce macro-level patterns that lend themselves to explanatory interpretations. For example, empirical models can accurately reproduce flight patterns of birds, even emergent ones, in the absence of theory explaining the patterns (but offering insights about the outcome to be explored). Mechanistic or "bottom-up" models, common in the biophysical sciences and some parts of the social science (e.g., economics), rely on theory-based deductive approaches. CAS science supports both approaches because its ontology explicitly represents the behavior of agents, for which theory exists and can be tested, while also providing environmental responses to that behavior and agents' responses to the changes in the environment (Fig. 2). This mechanistic and empirical blend opens opportunities to identify and explore integrated human-environment theory (Turner et al., 2020). CAS science has empowered computational social science, allowing researchers to explore social phenomena and test hypotheses by virtue of computer-based simulations of agents and their interactions (Bankes et al., 2002), nurturing a generative social science in which the dynamics are "grown" in the assessment stages (Epstein, 1999).

3.4. Enabling and evaluating processes and temporal progression

Revealing the temporal progression in a variable of interest (e.g., amount and spatial distribution of a certain resource or wildlife habitat) is important as projected patterns, if reliable, providing insights about the system's sustainability. For instance, dynamic habitat maps (e.g., Fig. S2, Supplemental file E) may inform the effectiveness of conservation policies. A "byproduct" of such temporal progression information is its usefulness for model evaluation. Many investigations evaluate models (mostly statistical models) based on their goodness of fit or the maximum likelihood. Modelers strike a balance between fitting the data (e.g., by adding more parameters or equations) and keeping the explanation as simple as possible (Rich, 1995), reflecting the long-time trade-off between generalizability and context (Janssen and Ostrom, 2006). Evaluation of CAS models, however, does not depend extensively on statistical performance. Rather, the CAS may provide insights into the viability of the mechanistic (e.g., cognitive, institutional, and/or social) processes accounting for CAS dynamics. In this case, the CAS informs us if the processes are justifiable or not—whether the system bears self-organization, becomes dissipative, or shows self-organized criticality (Manson, 2001).

CAS science assists in assessing outcomes, which represent states of agents and the environment at a certain level or temporal stage, and evaluate processes and temporal progression (Liu et al., 2015), asking whether the direction, magnitude, and significance of certain parameters are supported by existing theories. In essence, all the elements and arrows in Fig. 2 and Table S2 in Supplemental file C can be check points for SES documentation, assessment, or model evaluation.

As a "new kind of science", CAS science can leverage the patterns or trajectories ("data") generated by ABM simulations, assessing the extent to which such "data" align qualitatively and quantitively with empirical observations or theoretical frameworks. For instance, sustainability researchers may consider whether the univariate and bivariate statistics or regression coefficients based on such "data" are reasonable and supported by existing theory. Furthermore, the POM approach can escalate our confidence about our understanding of the CAS and its behaviors. Finally, the CAS ontology (Fig. 2) facilitates the development of new tools, platforms, or models, a high-priority research area in sustainability research (Liu et al., 2015). For instance, An and colleagues (An et al., 2020a) followed this ontology and developed a model to explain space-time dynamics among monkey behavior, habitat degradation, human resource collection activities, and nature reserve management policies in a Chinese nature reserve (Supplemental file E).

4. Leveraging AI to better understand SES

The four advantages identified for adopting CAS science and ABMs are built on prior knowledge about 1) the *structure and scales*, often hierarchical, at which agents are located, identified, and connected to one another and/or to the environment (Fig. 2), and 2) the *causal relationships* among the agents, the environment, and their behavior. Such knowledge is important in causal reasoning (Schlüter et al., 2023b). Yet from time to time, inadequacy of such knowledge exists, posing a problem for CAS modelers and sustainability scientists. AI, particularly its subfield of machine learning, can substantially empower CAS to address this problem (Cartwright, 2019; CSLI, 2020). The links between AI and CAS as well as their obvious implications for sustainability problems (e.g., elements in Fig. 2) warrant brief discussion, focusing on the benefits to detect mechanism(s) behind CAS and/or SES subject to sustainability challenges.

Through a process of data-based "training", machine learning can help derive CAS (or SES, the CAS equivalent in sustainability science) structures or processes (Section 4.1), or verify or rebut some hypothetical causal relationships or processes behind observed macro-patterns in the relevant CAS (Section 4.2). Many machine-learning methods allow for the training of complex models based on some high dimensional datasets. Such machine learning methods may range from the relatively basic linear models (e.g., standard linear regression) to more advanced models that can capture non-linear behavior (e.g., neural networks, especially deep learning). On the other hand, machine learning can be used to detect patterns in model output, which may help to evaluate the robustness of the model.

4.1. Use of AI to unveil system structure and scale(s)

Dealing with spatial, temporal, and organizational scales, including related scaling issues, remains a "grand challenge" for CAS modelers, requiring clear representation and matching of scales in relevant subsystems or individuals, variables, and processes (Elsawah et al., 2020). Just as in the Coleman's bathtub or boat framework (Coleman, 1990), a CAS modeler needs to know some "social facts" (e.g., institutions, social norms), a macro-level context corresponding to upper-level CAS (Fig. 2), which can regulate or affect the conditions or boundaries of individual actions, corresponding to focal CAS agents (Fig. 2). Such conditions or boundaries, once formed or changed, will lead to heterogeneous individual actions, which may finally form and reshape the starting macro-level context. Yet knowledge about the structure and this kind of macro-micro-macro interactions between agents and the environment may be a luxury in many instances. What if CAS modelers only possess data at specified spatial (e.g., focal and/or upper CAS), temporal (e.g., historic or current CAS), or organizational scale(s)?

Our answer is that AI, among many other alternative approaches, can help unveil—at least offer hints about—such structure, interactions, and scales. Advances in data science have yielded a wide variety of scientific methods, programming tools, and appropriate data infrastructures, facilitating analysis of new forms of data (including bigdata) in a scalable, efficient, and robust fashion. This advantage boosts AI's power to understand human intelligence and simulate how agents perceive, act, and react to other agents and/or changes in the environment(s) around them (Gil and Selman, 2019). One prominent aspect of AI features neural networks, which are comprised of nodes in different layers and their links to one another mimicking human and animal brain structures. Nodes can be understood as agents in CAS or actors in SES, while links are agent-agent or agent-environment relationships in CAS or SES (Cranmer et al., 2020; Kipf and Welling, 2016), which can be referred to the actors and arrows in Fig. 2.

Once sufficient data are provided and an appropriate model structure is chosen, the trained models, often with high predictive power, help to calibrate and/or validate CAS structure or processes better. Each agent or actor can be assigned with its own unique regression equation or

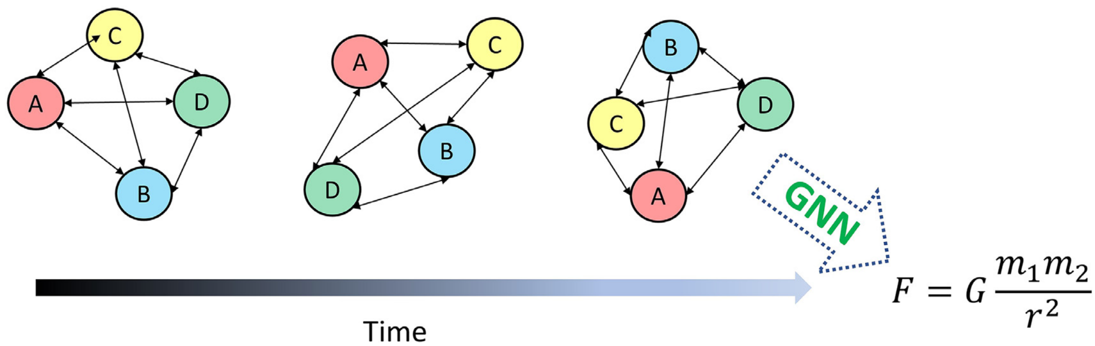

Fig. 3. Derivation of the Newtonian law of gravitational force. The process is based on data on particles (represented as circles of different colors) over time using a machine learning approach (Cranmer et al., 2020). F, G, m_1, m_2, and r represent the force between Particles 1 and 2, gravitational constant, the mass of Particle 1, the mass of Particle 2, and the distance between the two particles. The double arrows represent forces between particles. GNN represents graph neural network.

neural network links (Zhang et al., 2016). Understanding and envisioning agent behavior or mechanistic processes becomes a process of optimizing the neural networks for the agents.[6] Recently, machine learning has advanced dramatically, helping to uncover mechanistic processes. In a successful instance (Cranmer et al., 2020), a graph neural network model has been trained to derive the closed-form, symbolic expression of Newton's law of motion based on experimental data The Newton's law of motion can be derived through machine learning based on the mass, charge, geographic positioning information, and other information of all particles (corresponding to agents in Fig. 3) in the experiments. In other words, the machine learning approach ultimately produced a learned mathematical function that precisely replicates Newton's formula:

$$F = G\frac{m_1 m_2}{r^2} \quad (1)$$

where F, G, m_1, m_2, and r represent the force between Particles 1 and 2, the gravitational constant, the mass of Particle 1, the mass of Particle 2, and the distance between the two particles, respectively. Nothing is required as to prior knowledge regarding its form (Fig. 3). This example suggests AI's major potential to uncover laws or mechanisms in other domains, nourishing an AI-informed CAS and sustainability sciences. Expanding from the above example, A, B, C, D, and so on could be users (agents) of a "commons" resource (e.g., water resource), and arrows represent the power, interactions, and governance rules of these users in a certain SES. If we know some data of these agents (users) and the environment (e.g., the amount of renewable water, and the uses of the water), we are likely to derive the possible rules or mechanisms that are hidden but generate such data.

4.2. Use of AI to understand causality

One barrier that besets both sustainability and CAS sciences is the difficulty of detecting the most reasonable mechanism(s) behind the data or patterns observed, and particularly, identifying a set of justifiable rules applied to them (An, 2012; An et al., 2021; Cumming, 2008). The causal relationships behind the patterns or data can vary across studies and approaches (Schlüter et al., 2023b). Various AI methods, which contribute to better integrating "empirical analyses and process- or agent-based modeling", will enhance sustainability modelers' capacity to unravel "complex causal processes that affect sustainability" (Schlüter et al., 2023a). Below we use an example to show how AI can help detect causal relationships.

How will Mikania (*Mikania micrantha*)), an invasive vine species that may smoother and kill canopy trees, affect the habitat use of deer in Chitwan National Park and its buffer zone (Bhatta et al., 2021; Shrestha, 2016)? The literature is unclear on whether plant invasions are a consequence of deer browsing or occur independent of deer browsing (Blossey and Gorchov, 2017). Observational evidence for ungulate herbivory, however, indicates that browsing is a strong facilitator of exotic plant invasion. Suppose Mikania data, including GPS collar data of deer, exist over time. How can we derive deer behavioral rules with reference to Mikania?

Reinforcement learning (RL, an artificial intelligence algorithm) method, is used to figure out animal "decision" rules (Fig. 3; An et al., 2023), despite zero pre-knowledge regarding the causal relationship (or independence) between deer herbivory and Mikania invasion. Telemetry data (Panel A, Fig. 4) will be used as input to train the RL neural network (Panel B); the RL neural network, once trained, can then learn and establish a set of nodes and links, which can maximize a reward function with compliance to the state (largely data; Panel B). However, the established nodes and links are hidden. How can the modeler know these nodes and links? A regression tree (Panel C) can be leveraged, which translates the findings into a set of visible decision tree links (arrows in Panel C) and nodes (e.g., C1, C2, C3, d1, d2, d3 in Panel C). In turn, these nodes and links, with the aid of some fundamental domain knowledge, can be used and interpreted as meaningful and understandable mechanisms (Panel D). The node "if *Mikania* < 15 %" (within the blue box in Panel D) comes from the multiple nodes and links in the blue area of Panel C (modified from Fig. 2 in An et al. (2023)). Knowledge obtained this way, e.g., those "if…then…else if…then" statements that are translated from the hidden nodes and links, will likely represent the decision rules that deer use when roaming on the landscape.

4.3. Use of AI to process and use qualitative data

As pointed out by Clark and Harley (2020), "actors' behavior and decisions, especially with respect to choices about the future, are motivated less by accurate anticipations of the future than by collectively held narratives". Leveraging text narratives in whatever media in CAS / sustainability models can increase their potential to inform agent behaviors and/or verify outcomes in CAS (Chattoe-Brown, 2020) or trajectories related to sustainability. In Supplemental file D, if some "sadness" data can be collected from related tweets, ABM's rules or predictions can be better verified or falsified about disaster or rescue dynamics. For challenges and weaknesses in ABM verification and validation, we refer to (An, 2012; An et al., 2021; Manson, 2002; Wilensky and Rand, 2007; Zhang and Robinson, 2021).

Recent advances in natural language processing and mining qualitative data (e.g., ethnography input, social media texts, and other textual sources) have shown promise to reveal the underlying reasons or explanations for a human agent's behavior, or their stance towards a debatable issue or policy. Owing to rapid advances and the success-

[6] Models trained in this way are not many, and one reason might be the difficulty of training neural networks for so many agents. Another challenge hinges on the difficulty of interpretation: such "trained" models provide little or no understanding of the mechanisms governing the processes, like a "black box".

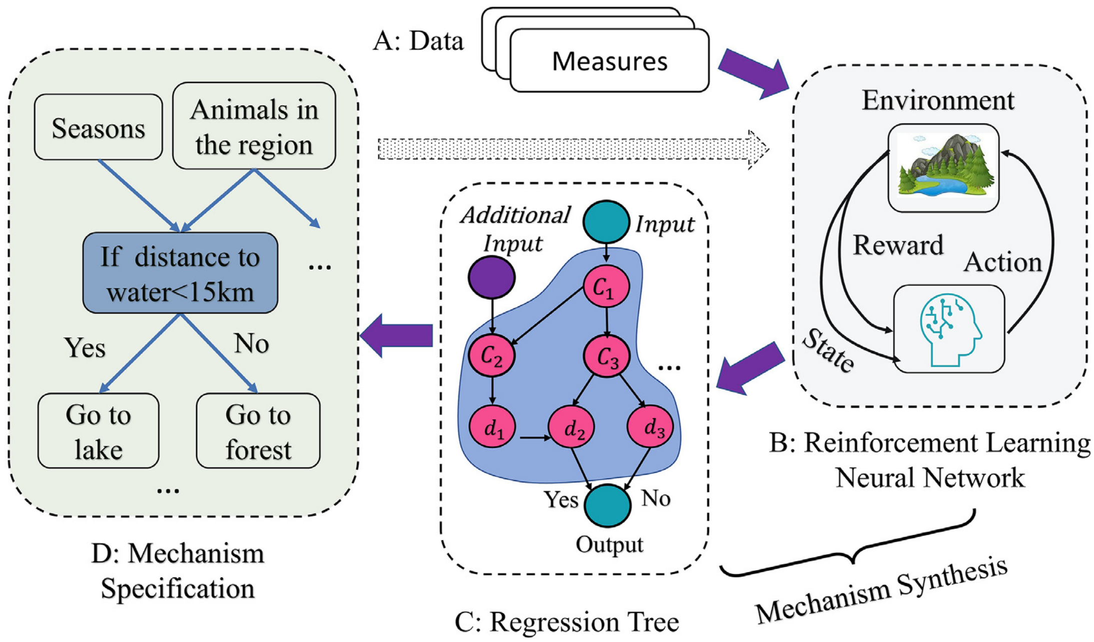

Fig. 4. Use of AI (reinforcement learning in particular) to decipher deer-environment relationships based on agent and environmental data (adapted from Fig. 2 of An et al. (2023)).

Table 1
Overview of the elements in the supplemental file to this article.

Element	Purpose and content	Page # *
A. The three essential elements in social-environmental systems	Introduction of the three common elements in social-environmental systems: actors, environment, and outcomes, their relationships, and exemplar references	1
B. The representation and ontology of complex adaptive systems	The ontology of agents and environment that is represented as a hierarchical CAS structure (Fig. 2 of main text) with time progression; the consistency between the ontology and sustainability science's dimensions	1–2
C. Literature search and review	The way, including search keyword and time frame, under which all the case studies in the realms of complex adaptive systems (CAS) science and sustainability science (SS) are selected (all cases shown in Tables S1 and S2 in Supplemental file C)	2–4
D. Use of non-traditional data to unfold dynamic patterns	An example of social-sensing analysis, which shows how Twitter (X) data can be used to unfold the dynamic patterns of emotions (e.g., anger, disgust, fear, joy, sadness, and surprise) in different topics related to a hurricane	4
E. ABM for Systems integration, scenario test, and space-time trajectories	An exemplar ABM that shows how human resource extraction and migration activities, affected by conservation payments, may interact with the Guizhou golden monkey (*Rhinopithecus brelichi*) habitat use in a Chinese Nature Reserve (An et al., 2020a)	4–5
F. Foraging behavior model for theory testing using ABM	Another exemple of an ABM investigates hunting outcomes under different conditions in the Mbaracayu Forest Reserve of Paraguay, including hunting strategies, group sizes, and mobility patterns (Janssen and Hill, 2016)	5–6

* Page numbers refer to those in the Supplemental materials.

ful application of deep neural networks in natural language processing (Bahdanau et al., 2015) and software engineering (Nguyen et al., 2018), it is now possible to accurately and effectively translate English text (e.g., in social media)—through developing an interactive deep learning-based system—into a list of relevant and sequential Application Programming Interfaces, which can be used to derive ABM rules or verify ABM predictions as noted in Supplemental file D. Table 1 below shows the major elements in the Supplemental file, which is uploaded as a supplement document.

5. Concluding remarks

Humanity is facing a range of unprecedented sustainability challenges. Sustainability science addresses these challenges through examinations that integrate by examining the integration of human and biophysical subsystems that give rise to them. It blends mechanistic and empirical modeling approaches to understand the dynamics of the social-environmental systems. CAS science affords significant opportunities in these efforts, as demonstrated by those engaged in CAS and ABM research to date (Anderies et al., 2019; Elsawah et al., 2020; Schlüter et al., 2023a). It offers sustainability researchers a unique perspective and the related tools to consider relevant agents, environment, and their interactions across hierarchical levels, various locations, or times.

While not the first assessment of the power of CAS and ABM to contribute to sustainability science (e.g., Elsawah et al., 2020; Lindsay et al., 2020; Schlüter et al., 2023a), three aspects of the possible synergy are identified here. First, CAS science's attention to mechanistic processes could substantially benefit sustainability science. For instance, the POM approach may help address many finality-challenges embedded in sustainability science. Second, the ABM approach offers a powerful tool for systems integration, for use of cross-scale and cross-disciplinary data and models, for model evaluation, and for providing an ontology and structure to examine SES sustainability challenges. Third and last, these positives are likely to be enhanced by AI of the digital revolution (with input from data science), providing the potential to advance understanding of the social-environment systems and posit the means to make them more sustainable.

This paper focuses on how CAS and ABM may contribute to sustainability science beyond their current uses. In addition, our take on these potential uses is influenced by our research interests, which include CAS and ABM for sustainability themes (human-environmental science more broadly), land system science, landscape ecology, and geography as well as our shared methods residing in mainstream science. Other sustainability researchers engaged in this science or following different topical interests and explanatory perspectives may have different views than those expressed here.

Our focus does not negate or downplay the benefits that sustainability researchers may contribute to CAS and ABM. The challenges existing in sustainability science (see Section 2.1), such as those identified by Clark and Harley (2020), potentially serve as opportunities for CAS and ABM. For instance, the progress made on governance and institutions of environmental resources, "deep" causes of land-use change, or biophysical feedbacks on community justice will surely help CAS researchers to comprehend and interpret emergent, even surprising, patterns that arise among agents in different human-environmental conditions. While consideration of this sustainability-to-CAS/ABM orientation lies beyond the scope of this article, it warrants attention, and has the potential to strengthen connections among various sustainability research communities.

Declaration of competing interests

The authors declare no conflict of interest. The funders had no role in the design of the study; in the collection, analyses, or interpretation of data; in the writing of the manuscript; or in the decision to publish the results.

CRediT authorship contribution statement

Li An: Methodology, Investigation, Funding acquisition, Data curation, Conceptualization. **B.L. Turner II:** Writing – review & editing, Conceptualization. **Jianguo Liu:** Writing – review & editing, Conceptualization. **Volker Grimm:** Writing – review & editing, Conceptualization. **Qi Zhang:** Writing – review & editing, Data curation. **Zhangyang Wang:** Conceptualization. **Ruihong Huang:** Data curation.

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Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.geosus.2024.09.011.

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