Review

Not peer-reviewed version

Agent-Based Complex Systems Science in the Era of Global Sustainability Crisis

Li An *, B. L. Turner II, Jianguo Liu, Volker Grimm, Qi Zhang, Zhangyang Wang, Ruihong Huang

Posted Date: 22 September 2023

doi: 10.20944/preprints202309.1571.v1

Keywords: social-environmental systems; agent-based complex systems; sustainability science; agent-based models; artificial intelligence; data science

Review

Agent-Based Complex Systems Science in the Era of Global Sustainability Crisis

Li An [1,2,*], B. L. Turner II [3], Jianguo Liu [4], Volker Grimm [5], Qi Zhang [6], Zhangyang Wang [7] and Ruihong Huang [8]

1 College of Forestry, Wildlife, and Environment, Auburn University, 602 Duncan Drive, Auburn, AL 36849, anli@auburn.edu.
2 International Center for Climate and Global Change Research, Auburn University, 602 Duncan Drive, Auburn, AL 36849, anli@auburn.edu.
3 School of Geographical Sciences and Urban Planning & School of Sustainability, Arizona State University, PO Box 875302, Tempe, AZ 85287-5302, Billie.L.Turner@asu.edu.
4 Center for Systems Integration and Sustainability, Michigan State University, East Lansing, MI 48823-5243, USA. liuji@msu.edu.
5 Helmholtz Centre for Environmental Research – UFZ, Department of Ecological Modelling, Permoserstr. 15, 04318 Leipzig, Germany, volker.grimm@ufz.de
6 Department of Geography, University of North Carolina at Chapel Hill, Chapel Hill, NC 27599, USA, qz@unc.edu.
7 Department of Electrical and Computer Engineering, The University of Texas at Austin, Austin, TX 78712, USA, atlaswang@utexas.edu.
8 Department of Computer Science and Engineering, Texas A&M University, College Station, TX 77843, USA, huangrh@tamu.edu.
* Correspondence: anli@auburn.edu; Tel.: 334-844-1028

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 Agent-based Complex Systems—ACS science—has a significant potential to handle such challenges. The advantages of ACS science for sustainability are addressed by way of identifying the key elements and challenges in sustainability science, the generic features of ACS, and the key advances and challenges in modeling ACS. Artificial intelligence and data science promise to improve understanding of agents' behaviors, detect SES structures, and formulate SES mechanisms.

Keywords: social-environmental systems; agent-based complex systems; sustainability science; agent-based models; artificial intelligence; data science

1. Introduction

The Anthropocene witnesses unprecedented conditions and challenges about human-environment relationships [1,2]. 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 [3,4] to the consequences of consumption on the functioning of the Earth system [5]. 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 [6–8]. This search, in turn, has given rise to sustainability science, a use-inspired science seeking to advance understanding about critical elements that promote sustainable development [9–11]. It constitutes "a new social contract for science" [12], akin to agricultural or medical research [10], 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 [11].

Human-environment interactions reside at the core of the sustainability science, and are addressed as social-environmental systems (SESs: aka social-ecological systems or coupled human and natural systems [13,14]), which behave as complex adaptive systems [15]. Comprehensive synthesis articles [9–11,16,17] and online repertoires [18,19] indicate that SES maintain at least three overarching elements: actors, environment, and outcome (detail in Appendix A) [10].

Several central challenges emerge in sustainability science, pursuant to its goal of sustainable development [11], 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 challenges in question. Here, we focus on several broad challenges to sustainability science in which Agent Based Complex Systems (ACS) science (ACS science hereafter), as labeled by Grimm and colleagues [20], may provide potentials to resolve, especially in light of Artificial Intelligence (AI; AI hereafter). ACS science is the systems science that studies "dynamic networks of many interacting agents" [20] 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 (detail in next section). AI, as the process of perceiving, synthesizing, and inferring information by machines [21], may substantially empower ACS science when addressing sustainability challenges. In particular, we will 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 the SES that sustainability science examines. These SES are highly diverse in kind and in the problems applied to them. Likewise, they are complex given the dimensions of factors and relationships comprising the systems [11]. The heterogeneity of elements examined at the lower and focal levels and across time draw attention to place-based or context specific outcomes, and hence resolution strategies, owing to the SES complexities, although it is understood that some kind of general processes operate throughout the system [7,11]. Given the high dimensionality and complexity of sustainability challenges, "silo approaches" [17] 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 [22] (e.g., human-nature nexus and telecoupling). At the same time, sets of metrics capturing the dimensionalities involved have been proposed, such as ecosystem/environmental services, environmental footprints, planetary boundaries, and inclusive wealth [16,23]. In perhaps the broadest framing, Clark and Harley propose that the spatial dynamics of human-environmental interactions at the mesoscale can serve as the integrator of the heterogeneity of lower-level dynamics and the relatively persistent, macro-scale patterns and processes operating on the SES [11]. Third, choosing among alternative theories or mechanisms to explain or project human decision-making or actions is a serious challenge. Alternative theories of resource uses may yield highly divergent or similar outcomes, with none outperforming the others in terms of robustness and validity [24]. Fourth and last, sustainability research and applications must enable and evaluate processes and temporal progression. 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 [25], becomes a must.

These challenges undergird our argument that ACS science, especially in the light of AI, may provide numerous opportunities for sustainability science. However, the sustainability science community is relatively unfamiliar with ACS science and its ABM methodology (detail in Section 2.2). The overarching goal of this review article is to illustrate the concept of ACS, its major methodology of agent-based modeling, new opportunities arising from AI, and their unique contribution to addressing the above sustainability challenges. We envision that ACS and

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 22 September 2023 doi:10.20944/preprints202309.1571.v1

sustainability sciences can be integrated, with strong possibilities of leading to breakthroughs in understanding and for application of sustainability problems.

2. Contribution of ACS Science to Addressing Sustainability Challenges

2.1. Handling the high dimensionality and complexity challenges

ACS Science provides a comprehensive, complex systems framework that can address the high dimensionality and complexity challenges in sustainability science. Compared to Complex Adaptive Systems [26] or Agent Societies [27] to which ACS are similar to, ACS emphasize the pivotal role of individual actors (i.e., agents in ACS) or entities (objects) that make choices (decisions) and/or act in order to pursue a certain goal [28]. Agents exist within ACS and interact with one another (Figure 1, dashed arrows) and with the environment. Agents possess different degrees of autonomy, proactivity, and intellectual capabilities, such as memory, knowledge, reasoning, learning, social capital, and adaptation. 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 [29]. This representation builds on a unique ontology (Figure 1) in which real-world actors are represented as heterogeneous, individual agents that comprise ACS and generate the interactions in question [30,31]. This ontology of methodological individualism represents a shift from understanding aggregate agent features and/or relationships to the individuals and micro-level processes (including interactions) that constitute and explain such aggregate features (detail in Appendix B). Given the features in this ontology (Figure 1), ACS science offers a comprehensive, complex systems framework, which can guide sustainability scientists and practitioners from the following perspectives.

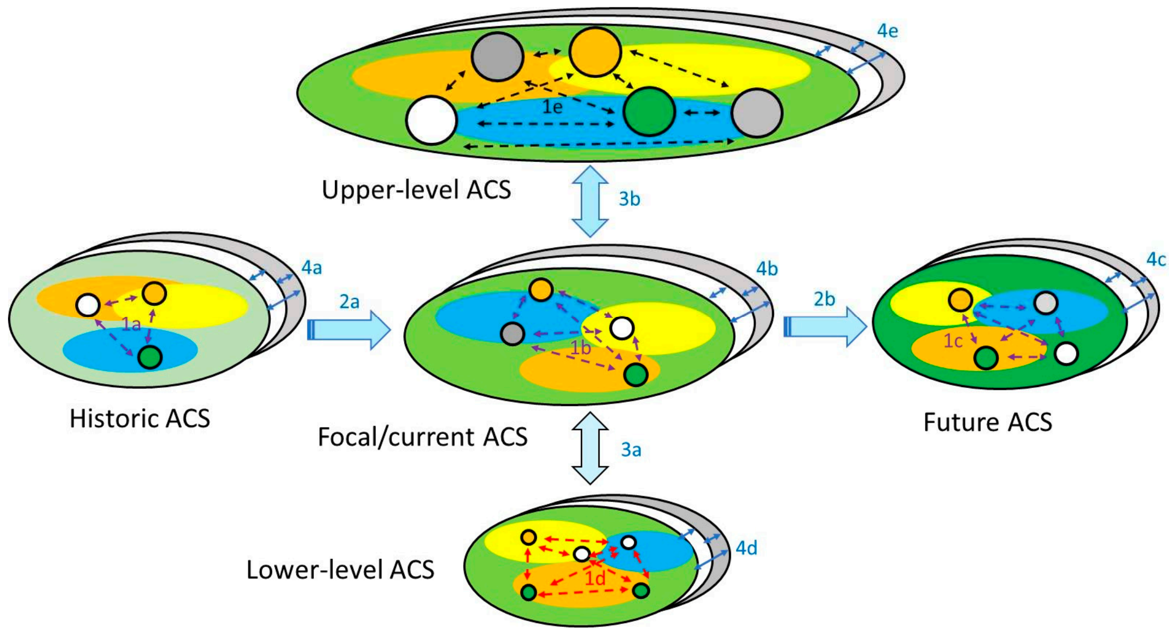

Figure 1. The ontology of agent-based complex systems (ACS). Circles and ovals represent agents and the environment, respectively, while arrows of different colors and shapes represent heterogeneous interactions or influences between various ACS elements. The numbers and letters represent interactions among agents and those among ACS, respectively.

First, social-environment systems under sustainability challenges can be examined in a hierarchical structure, where agents at one level or location may affect and be affected by agents at other levels or locations. To demonstrate the applicability and usefulness of this hierarchical structure, we performed a literature survey of empirical studies in both ACS and sustainability sciences (detail in Appendix C). We found that agents affect one another across lower-, focal-, and upper-levels; for example, individual migrants (lower-level agents) affect their households (focal agents) through sending back remittances [32], wastepaper markets (upper-level agents) affect decisions of wastepaper suppliers and recyclers (focal-level agents) [33]. For more examples, see Table S1 in Appendix C (under the lower-, focal-, and upper-level agent subcategories) and Appendix E, where individual monkey agents and monkey group agents affect each other across focal- and upper-levels.

Second, the importance of tracking (to a large degree) the behavior of autonomous, heterogeneous, and decision-making agents should be appreciated in SES. For instance, tracking movement of prey animals, predator animals, and hunters makes the ACS related simulation as realistic as possible: they encounter, hunt, or predate on the heterogenous landscape at certain times. This way, the simulation gives rise to meaningful results when alternative behavioral models are plugged in the agent-based model (ABM), testing the reliability of various theories of social behavior of hunter–gatherers behind these behavioral models (Appendix F).

Third, exploration of sustainability challenges should be administered in a dynamical, progressive way. This suggests that environmental conditions at earlier times may constrain those at current time, which may in turn further constrain those at future times. In this regard, there exist a plethora of case studies regarding the impacts of historic precipitation, disasters, fires, local weather conditions, and land use on the current environment (Table S1 under historic, focal, and future environment subcategories). Similarly, adjacent or distant environments may affect and be affected by the environment at the same level through various mechanisms such as the telecoupling effect [34] (Table S1 under the Same level (adjacent/distant) environment subcategory).

Fourth, decisions or actions of agents at one time or location may influence their own and other agents' decisions and/or actions, which may translate to system-level events and/or emerging outcomes at later times or other locations. Abundant 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 and ACS (see Table S1 under several agent-agent interaction subcategories); more discussion is in Section 2.4.

Fifth, at the system level, attention should be paid to mutual influences between SES (or ACS) across different levels, between parallel SES (ACS), or among different times. For instance, to project future human migrations and changes in the environment, Kniveton and associates point out that the interactions between parallel ACS 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 [35]. More examples about system-level SES/ACS interactions are presented in Table S1 (under various ACS-ACS interaction subcategories).

Finally—as a result of all the above points—this ontology provides a framework that captures the essence of many SES processes and dynamics (e.g., adaptive decision-making and the co-evolutionary aspect of ACS or SES). It guides sustainability interests in the formulation of goals (e.g., focus on focal-level alone or at focal-, lower-, and upper-levels), data collection (e.g., collect data at one time or multiple times), and analysis and modeling (e.g., perform cross-sectional data analysis, time series analysis, or simulation).

2.2. Providing an effective platform for systems integration

The modeling advances of ACS 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 in sustainability science; see Appendix A), attributes and/or traits, and behaviors of the agents should be included at each level of the corresponding ACS or SES?
- Environment: what attributes and processes should be included (especially those affected by and feed back to affect agents) at each level? In ACS, 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 can be the environment.

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 22 September 2023 doi:10.20944/preprints202309.1571.v1

- Agent-agent and agent-environment interactions: what relationships (expressed as rules, influences, or actions) among agents 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 [i]. This complexity includes surprises, path dependence, nonlinearity, self-organization, contingency, emergence, multifinality, and equifinality (for definitions see Liu et al. [13] and An [37]).

Sustainability science examines human-environment relationships in which actors/agents are people or people groups and the environment is the biophysical world. It seeks to understand the interactions between the two subsystems, which, more often than not, requires attention to components and interactions within or between subsystems. It is also open to applications of various methods and models, especially those that can handle integration among the components of SES [38]. ACS 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 [39], partial differential equations [40–42], cell-based stochastic modeling [43], and structural equation modeling [44] are not uncommon (for detail see Table S1). Regardless of the range of agents entertained, ACS 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 [45]). Significantly, agent-based modeling (ABM), as a prime ACS method and tool (e.g., credited to do "a new kind of science" [46]), provides a way to fuse the deductive-mechanistic and the inductive-empirical approaches that pervade different pathways toward understanding and envisioning ACS, earning it the moniker of a "third way of doing science" [47] (see endnote [ii] for more discussion).

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 [16]. Mimicking the realistic (though tailored and simplified) structure and processes of the system under investigation (Figure 1), ABM seeks to "translate" real-world actors, environment (e.g., forestland), and constraints (e.g., land use regulations; Figure 1) 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) [49] (see the exemplar ABM in Appendix E). ABMs are powerful when modeling learning and adapting processes [31,50,51], accounting for heterogeneity, bounded rationality and incomplete knowledge/information, and nonlinearities [52,53], and exploring many complexity features such as path-dependence, abrupt changes, and critical thresholds, among others [13,37].

ABMs have been widely developed and used in ACS studies to address problems confronting social, environmental, and social-environmental systems since the 1990s [55,56]. These endeavors have generated a rich legacy of ABM methodology, such as the Overview, Design concepts, Details (ODD) protocol for model documentation [57] and the Pattern-oriented Modeling (POM) approach [58] for model validation. At the same time, ABM endeavors have enriched the literature in sustainability science in terms of modeling human behavior [24,31] (e.g., the frameworks for Belief-Desire-Intentions and physical, emotional, cognitive, and social factors [27,59]), exploring how adaptive behavior, abrupt changes, crises or disasters, and critical transitions may generate surprising patterns in the corresponding SES [13,53,60], life cycle assessment [61,62], and modeling emergent macro-level outcomes and pathways under various policies or interventions [49,53,63,64].

A milestone in the sustainability science and ABM nexus was a 2006 special issue of *Ecology and Society* [45] addressing various empirical methods by which ABMs were empirically tested for SES. Subsequently, ABMs applied to sustainability problems have significantly increased, although they comprise only about 1.24% of all sustainability science publications in 2021 (Figure 2). Among the 29 ACS cases in our literature survey, 22 use ABM as the major method, while among the 32 sustainability science cases, only nine use ABMs (Table S1 in Appendix C). Aside from a variety of

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 22 September 2023 doi:10.20944/preprints202309.1571.v1

challenges in developing and employing ABMs (e.g., sharp learning curve, high data demand, programming difficulties) [31,52,55], the relative unfamiliarity of ACS science and ABMs in the sustainability science community highlights the timeliness and importance of this article.

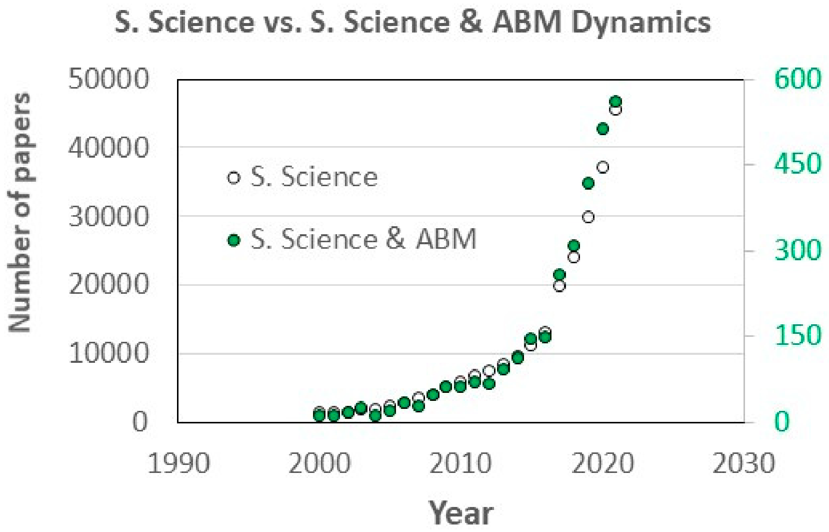

Figure 2. The publications addressing sustainability science (left Y-axis) vs. those using ABMs (right Y-axis) to address sustainability problems since 2000 (S. Science = sustainability science; for data search detail, see the endnote [iii]).

2.3. Handling alternative pathways or theories in sustainability

ACS science has been wrestling with "finality" related challenges, which also abound in sustainability problems. Equifinality—a macro-level pattern can be generated through different pathways from micro-level processes [65]—confronts the search for mechanistic processes. In ACS science, for instance, cooperation or betrayal in the Prisoner's Dilemma can emerge from tit-for-tat retaliation [66], strong reciprocity [67], and group selection [68], among other strategies [69]. 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 [55].

The Pattern-Oriented Modeling approach [58,70], overlapping with Approximate Bayesian Computing [71] in ACS, offers a possible means to address the "finality" challenges. 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 ACS. 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 high synergy between ACS and sustainability sciences hitherto discussed, we posit that despite its rare application in sustainability science, POM may prove useful to uncovering many sustainability related mechanisms. We refer to the example of foraging behavior model for theory testing using ABM (Appendix F).

Given the reflexivity of human agents, the social sciences tend to approach the dynamics of the social subsystem in multiple, probabilistic ways, commonly applying both quantitative and qualitative methods. Empirical models use evidence to explore outcomes and plausible, inductively derived explanations. 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. ACS 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 (Figure 1). This mechanistic and empirical blend opens opportunities to identify and explore integrated human-environment theory[38]. ACS 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 [72], nurturing a generative social science in which the dynamics are "grown" in the assessment stages [73].

2.4. Enabling and evaluating processes and temporal progression

Revealing temporal progression in the variable of interest (e.g., amount and spatial distribution of a certain resource or wildlife habitat) is important as projected patterns, if reliable, provide insights about the system's sustainability. For instance, the dynamic habitat maps in Figure S2 (Appendix E) may inform whether the conservation policy is effective. 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 [74], reflecting the long-time trade-off between generalizability and context [45]. Evaluation of ACS models, however, does not depend extensively on statistical performance. Rather, the ACS may provide insights into the viability of the mechanistic (e.g., cognitive, institutional, and/or social) processes accounting for ACS dynamics. In this case, the ACS informs us if the processes are justifiable or not.

ACS 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 [16], asking whether the direction, magnitude, and significance of certain parameters are supported by existing theories. In essence, all the elements and arrows in Figure 1 and Table S1 can be check points for SES documentation, assessment, or model evaluation. As the "new kind of science", ACS science can leverage the patterns or trajectories ("data") generated by ABM simulations, evaluating whether and how much such "data" qualitatively and quantitively agree with empirical observations or theory. 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 ACS and its behaviors. Finally, the ACS ontology (Figure 1) facilitates the development of new tools, platforms, or models, a high-priority research area in sustainability research [16]. For instance, An and colleagues [54] 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 (Appendix E).

3. Opportunities from Artificial Intelligence to better understand SES

Our last section illustrates the four major advantages of adopting ACS science to address sustainability challenges. One barrier that besets both sustainability science and ACS science is the difficulty of detecting most reasonable mechanism(s) behind the data or patterns we observe, and particularly, identifying a set of justifiable rules [31,50,55]. Artificial intelligence (AI), particularly its subfield of machine learning, can substantially empower ACS [75,76]. Rather than elaborating on AI in detail, this article only aims to show the links between AI and ACS as well as their obvious implications for sustainability problems (e.g., elements in Figure 1). For this reason, our description of AI is brief, focusing on its benefits on detecting mechanism(s) behind ACS and/or SES subject to sustainability challenges.

Through a process of "training", machine learning can help derive ACS (or SES, the ACS equivalent in sustainability science) structures or processes that verify or rebut the underlying structures, mechanisms, forces, and/or processes behind macro-patterns in the relevant ACS. 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.,

 doi:10.20944/preprints202309.1571.v1

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.

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 [77]. 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 ACS or actors in SES, while links are agent-agent or agent-environment relationships in ACS or SES [78,79], which can be referred to the actors and arrows in Figure S3 (Appendix G). 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 ACS structure or processes better. Each agent or actor can be assigned with its own unique regression equation or neural network links [80]. Understanding and envisioning agent behavior or mechanistic processes becomes a process of optimizing the neural networks for the agents [iv]. Recently, machine learning has advanced dramatically, helping to uncover mechanistic processes. In a successful instance [79], a graph neural network model has been trained to derive the closed-form, symbolic expression of Newton's law of motion based on experiment data (detail in Appendix G).

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 successful application of deep neural networks in natural language processing [81] and software engineering [82], 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 Appendix D.

As pointed out by Clark and Harley [11], "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 ACS / sustainability models can increase their potential to inform agent behaviors and/or verify outcomes in ACS [83] or trajectories related to sustainability. In Appendix 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.

4. Concluding Remarks

Humanity is facing a range of unprecedented sustainability challenges. Sustainability science addresses these challenges through examinations that integrate the 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. ACS science affords significant opportunities in these efforts. It offers sustainability researchers a unique perspective and the related means to consider relevant agents, environment, and their relationships at hierarchical levels, various locations, or times.

The contribution of this article lies in the following three aspects. First, this article points to many ACS efforts of seeking mechanistic processes, which could substantially benefit sustainability scientists. For instance, the POM approach may help better address many "finalities" challenges in sustainability science. Second, the ABM approach could offer 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 when examining a certain SES subject to sustainability challenges. Third and last, these positives are likely to be enhanced by artificial intelligence of the digital revolution

 doi:10.20944/preprints202309.1571.v1

(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.

Supplementary Materials: The following supporting information can be downloaded at the website of this paper posted on Preprints.org. Figure S1: Dynamics of emotions during Hurricane Harvey in Houston, TX, August 25–30, 2017; Figure S2: Differences in monkey habitat use density; Figure S3: Derivation of the Newtonian law of gravitational force; Table S1: Examples of components in agent-based complex systems (ACS) science and sustainability science (SS) and cases (examples) in literature.

Author Contributions: Conceptualization, L.A., J.L., and B.L.T.; methodology, L.A., V.G., Q.Z., Z.W., R.H.; Writing—original draft: LA, Writing—review & editing: All authors; project administration, L.A.; funding acquisition, L.A. All authors have read and agreed to the published version of the manuscript.

Funding: This research was funded by the National Science Foundation (NSF) through the Method, Measure & Statistics and Geography and Spatial Sciences (grant number BCS #1638446) and the Dynamics of Integrated Socio-Environmental Systems programs (grant number BCS 1826839 and DEB 1924111).

Acknowledgments: We thank San Diego State University and Auburn University for financial and logistic support.

Conflicts of Interest: 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.

Appendix A. The three essential elements in social-environmental systems.

Actors. Be they individuals, companies, governments, or other entities, actors (a) maintain and are regulated by a variety of attributes: values, knowledge and information, institutions (rules/policies, norms, culture, beliefs [19]), power (the ability of actors to affect the beliefs or actions of other actors [84]), and goals; and (b) make decisions, act, or interact with other actors and the environment in their efforts to achieve corresponding goals. Actors, of course, operate within "environments"—such as social, cultural, political, or eco-physical—variously identified by different research communities.

Environment. The bio-geophysical conditions of the earth constitutes the environment for research communities examining SESs, with attention to natural capital and environmental (or ecosystem) services [85]. These conditions, from ecosystems to the Earth system, are shaped by what actors do and feed back to them, either enhancing or constraining, but affecting what actors do now and in the future.

Outcomes. Human-environmental conditions that follow from the interactions of the actors and the environment constitute the outcomes in question, including pathways, trajectories, and emergent patterns. They tend to be measured by an array of anthropogenic and environmental capitals for which various metrics exist [23].

Appendix B. The representation and ontology of agent-based complex systems

The agents and environment ontology is represented as circles and ovals, respectively in Figure 1. The agents and environment maintain heterogenous characteristics (represented as different colors of circles and of ovals), considered at the lower-, focal-, and upper-levels as identified by Clark and Harley [11]. The upper-level agents and environment provide the context and constraint for the behavior and dynamics of the system at the focal level. The focal-level is that of the major interest for the study in question, which is the level in which data collection, analysis, and modeling are focused on (although—in many instances—some substantial efforts also go to the lower-level). The lower-level offers details and processes that explain the focal-level behaviors and dynamics. Interactions happen between agents; such interactions are symbolized as purple, red, and black dashed arrows, representing interactions among agents at focal- (Arrows 1a, 1b, and 1c for historic, current, and future ACS), lower- (Arrows 1d), and upper-levels (Arrows 1e), between different times (the one-way, bold arrows representing influences from the past and into the future, arrows 2a and 2b

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 22 September 2023 doi:10.20944/preprints202309.1571.v1

respectively), between the focal level and its lower- or upper- levels (Arrows 3a and 3b respectively), and between the ACS under consideration and other adjacent or distant ACS at the same level (Arrows 4a, 4b, and 4c represent cross-ACS interactions at historic, current, and future times; Arrows 4d and 4e represent cross-ACS interactions at lower- and upper-levels). For the environment at each level (ovals with boundary), there are sub-regions or sub-environments (the boundaryless ovals), representing environmental heterogeneity.

The representation of ACS in Figure 1 is consistent with the framing of the dimensions of integrated approaches in sustainability science proffered by Clark and Harley [11], but substitutes lower, focal, and upper levels (hierarchical or spatial) for their micro, meso, and macro levels. This consistency is also demonstrated in the literature survey of empirical studies (Table S1 in Appendix C). In these studies, the ACS cases are those that reflect Figure 1, while the sustainability science (SS) cases are those in which agents are people or people groups and the environment is (or involves) a biophysical environment. The literature survey shows that 1) the agents (circles), environment (ovals), and interactions or relationships (arrows) as shown in Figure 1 can be identified in all these empirical studies regardless of whether it is an ACS or SS case. 2) The major methods employed in ACS and sustainability sciences, if only partially identified, belong to two different methodological spectrums, but with sizeable overlapping in the use of agent-based modeling (ABM). 3) Sustainability science's synergy with ACS science is illustrated by allowing for agents, for example, people or households, to influence or interact with the biophysical environment. Many cases, if qualifying both ACS and sustainability sciences, are identified as ACS science (marked with an asterisk mark).

Appendix C. Literature search and review

We conducted a literature search and review of research articles in the realms of agent-based complex systems (ACS) science and sustainability science (SS). The goals of this search and review are 1) to establish and solidify the ontology of agent-based complex systems (Figure 1), and 2) to show the applicability of this ontology in sustainability science. The knowledge of all authors about ACS science helped establish an earlier version of the ontology, which was enhanced as we read the papers that were selected. Finally, we finalized the ontology to its present form (Figure 1) and selected cases that reflect its various components (Table S1). The papers were selected from a Scopus-based search (see below) for ACS science and SS cases. The authors' personal archives of papers in ACS and SS, along with a "snowball" search based on papers that have been chosen, also contributed to this search and review. In several cases, we included more than one case for some of the components to provide a clearer idea on the conceptual meanings. The definition of *focal-level agents* depends on the level of focus in the research design of a study, e.g., a focal agent can be a household between the levels of people and community, or it can be a country between the levels of a state and the world. We obtained the major method(s) used in all the retained cases.

We chose Scopus to search for articles and select representative candidates. Scopus, produced by the Elsevier Company, is the largest bibliographic database that covers 14,000 STM (i.e., Science, Technology, and Mathematics) and social science titles from 4,000 publishers [86]. We used the Advanced Search mode with Boolean operators and nesting functions to search articles. According to Scopus, subject areas can be divided into four major categories, including health sciences, life sciences, physical sciences, and social sciences. There are totally 25 subject areas[1] falling within these

---

[1] The specific subject areas with their abbreviations under the four major categories are as follows. Health Sciences (5): Medicine (MEDI), Nursing (NURS), Veterinary (VETE), Dentistry (DENT), Health Professions (HEAL). Life Sciences (5): Agricultural and Biological Science (AGRI), Biochemistry, Genetics and Molecular Biology (BIOC), Immunology and Microbiology (IMMU), Neuroscience (NEUR), Pharmacology, Toxicology and Pharmaceutics (PHAR). Physical Sciences (9): Chemical Engineering (CENG), Chemistry (CHEM), Computer Science (COMP), Earth and Planetary Sciences (EART), Energy (ENER), Engineering (ENGI), Environmental Science (ENVI), Mathematics (MATH), Physics and Astronomy (PHYS). Social Sciences (6): Arts and Humanities (ARTS), Business, Management and Accounting (BUSI), Decision Sciences (DECI), Economics, Econometrics and Finance (ECON), Psychology (PSYC), Social Sciences (SOCI).

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 22 September 2023 doi:10.20944/preprints202309.1571.v1

four categories. For SS cases, we chose two of the most relevant subject areas, which are Environmental Science (ENVI) under Physical Sciences and Social Sciences (SOCI) under Social Sciences. For ACS, we covered all the 25 subject areas. We acknowledged that some studies in ACS can fall within the SS domain due to the overlaps between them (e.g., agent-based simulations that were used to answer sustainability questions). In some cases, if a study relies on a theoretical foundation described in a previous publication (before 2000), we also retained that earlier publication as a reference associated with the study case.

For SS studies, we used the terms of "sustainable", "sustainable development", and "sustainability" that appear in titles to search article candidates. We set the time frame back to 2010, namely 2010-present (as of December 2022) and set language to "English". We limited the document type and the source type to "Article" and "Journal", respectively, selected those with keywords of "Sustainable Development" or "Sustainability", and limited the search to the most relevant areas, which is Environmental Science. The final query is refined as follows: TITLE ("sustainable") OR TITLE ("sustainable development") OR TITLE ("sustainability") AND PUBYEAR > 2009 AND PUBYEAR < 2023 AND (LIMIT-TO (SRCTYPE , "j")) AND (LIMIT-TO (PUBSTAGE , "final")) AND (LIMIT-TO (DOCTYPE , "ar")) AND (LIMIT-TO (SUBJAREA , "ENVI")) AND (LIMIT-TO (LANGUAGE , "English")) AND (LIMIT-TO (EXACTKEYWORD , "Sustainable Development") OR LIMIT-TO (EXACTKEYWORD , "Sustainability")). The query resulted in 30,414 documents, which were then sorted by citations. We read through the titles and abstract from the most cited article and retained those most relevant to the essence of human-environment interactions as the core of SS and its major elements (e.g., actors, environment, and outcomes). We adopted the "snowball" approach (both backwards and forwards) to search articles with specific cases that may reflect at least one component of interest in the ontology. We summarized all the selected cases that can explicitly or implicitly manifest the finalized ontology.

Since ACS studies may cover a variety of research fields, we search candidate articles falling in different subject areas defined by Scopus. Note that agent-based modeling (ABM) is not the only approach in ACS studies. Alternatively, approaches such as Cellular Automata are also capable of capturing feedbacks between agents. We addressed such methodological diversity by considering a balanced review of cases both with and without using ABMs, particularly for those in ACS. We used the terms of "agent-based", "multi-agent", "cellular automata", "system dynamics", and "partial differential equations" that appear in titles to search article candidates. The other conditions are similar to those used for SS studies, except for not defining keywords. Therefore, the query is as follows: TITLE ("agent-based") OR TITLE ("multi-agent") OR TITLE ("cellular automata") OR TITLE ("system dynamics") OR TITLE ("partial differential equations") AND PUBYEAR > 2009 AND PUBYEAR < 2023 AND (LIMIT-TO (SRCTYPE , "j")) AND (LIMIT-TO (PUBSTAGE , "final")) AND (LIMIT-TO (DOCTYPE , "ar")) AND (LIMIT-TO (LANGUAGE , "English")). The query resulted in 24,869 documents, covering 27 subject areas[2]. We grouped these article candidates by the subject areas and again sorted them in each subject area. Starting from the most cited article candidate and using the "snowball" approach, we retained and summarized study cases that can reflect at least one component of the finalized ontology (Table S1).

Appendix D. Use of non-traditional data to unfold dynamic patterns

Social media is considered as a means to analyze knowledge-sharing behaviors between software developers and users in the process of engineering software requirements [87]. Recently, increased research on emotion analysis [88–90] and emotion cause analysis [91–93] based on social-

[2] Computer Science (10,818), Engineering (10,312), Mathematics (8,120), Physics and Astronomy (2,697), Environmental Science (2,505), Social Sciences (2,501), Materials Science (1,652), Business, Management and Accounting (1,385), Energy (1,365), Decision Sciences (1,166), Biochemistry, Genetics and Molecular Biology (871), Agricultural and Biological Sciences (826), Medicine (801), Chemistry (761), Chemical Engineering (754), Economics, Econometrics and Finance (745), Earth and Planetary Sciences (698), Multidisciplinary (578), Neuroscience (551), Arts and Humanities (265), Pharmacology, Toxicology and Pharmaceutics (205), Psychology (176), Immunology and Microbiology (156), Health Professions (75), Nursing (36), Veterinary (27), Dentistry (7).

media texts, adopting both traditional machine-learning methods and recent deep-learning approaches, has been undertaken.

In a recent social-sensing analysis of the impacts of disasters [94], it has been shown that Twitter data are useful to unfold the dynamic patterns of emotions (e.g., anger, disgust, fear, joy, sadness, and surprise) in different topics related to a hurricane (Figure S1), which falls within the class of "data-driven models" [95]. Also research has been invested on integrating social sensing with remote sensing [96]. When we infuse such data into sustainability science, for example for fire hazard or land use and land cover change analysis, we may better explain why a fire control regime or land use policy may work or fail based on people's emotion patterns, values, or worldviews.

Appendix E. ABM for Systems integration, scenario test, and space-time trajectories

An et al. developed an ABM to show how human resource extraction and migration activities, affected by conservation payments, may interact with the Guizhou golden monkey (*Rhinopithecus brelichi*; a shy species that avoids humans) habitat use on a 419 km^2 landscape [54]. This study features 1) multiple disciplinary data organized at various spatial, organizational, and temporal scales: household survey data at the individual people and household levels (yearly basis), monkey observations and data at the monkey individual and group levels (5 day basis), vegetation and land use maps (5+ year basis), and so on; 2) models and knowledge from different disciplines: sociology (human migration, participation in conservation programs), demography (e.g., childbearing, marriage, death), ecology (vegetation growth), and primatology (monkey behavior); and 3) different livelihood strategies affected by conservation policies at various temporal scales: local villagers can be paid to return farmland to forestland (by year), migrate out (by year), remain at home (by day), or go to mountains for resource (fuelwood and fodder) extraction (by day). The ABM assigns the above data to different agents (e.g., income data to household agents and habitat use to monkey agents), lets the data update at the corresponding temporal scales (e.g., income changes by year and monkey habitat use changes by days), and puts the agents on the landscape with geographic coordinates recorded over time. In this way, a spatiotemporally explicit ABM is built, allowing people agents to experience demographic (e.g., bear children, marry, migrate) and livelihood (collect fodder or fuelwood) processes on the space, monkey agents roam on the landscape (represented as pixels of 300 × 300 m), and environment is assigned to various land use or cover types. Thus, the ABM integrates multiple disciplinary / scale data (putting data as attributes of agents and update them at various temporal scales), knowledge (using it as agents' behavioral rules), and policy (using it to build scenarios), making the monkey agents to escape when "encountering" the people agents. As a result, space-time trajectories (maps) can be generated for sustainability explorations. The map below shows the degree of habitat degradation (increasing from yellow to red) at years 10 and 20 (Figure S2), based on local people receiving 0, 270, and 540 yuan/mu (Chinese currency; 1 yuan = 0.14 USD in 2020; 1 mu = 1/15 hectare) from the conservation program.

Appendix F. Foraging behavior model for theory testing using ABM

Janssen and Hill use an ABM to explore what hunting outcomes emerge under different conditions in the Mbaracayu Forest Reserve of Paraguay, including hunting strategies (solitary vs group), group sizes, and mobility patterns (varying camp size and movement frequency) [97]. Prey animals (one type of agent) move around with their density correlated with vegetative resources; surviving animals reproduce on a yearly basis. Comparing simulation outcomes with real data (e.g., frequency distribution of total meat obtained per day by a hunter, percent of time searching for prey), they found that hunters (another type of agent) achieved hunting outcomes that best match the observed data when adopting a strategy identified as the Camps with Coordinated Search and Cooperative Pursuits (CCSP). This strategy is closely aligned with Optimal Foraging Theory of social behavior of hunter–gatherers, suggesting its usefulness under complex conditions. The modeling complexity involves heterogeneity, feedback, and adaption: the environment is characterized by time-variant returns, and hunting decisions change over time, hinging on what has happened when and where resources are exploited, and so on. In addition, cooperative hunting did not generate

Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 22 September 2023 doi:10.20944/preprints202309.1571.v1

considerable increases in hunting gains compared with independent hunting. Therefore, the authors posit that group (community) living may arise not from hunting rewards but from other types of social support such as predator protection and cooperative childcare. Overall, this use of the ABM demonstrates its viability in identifying which theory of human-environment interactions appears to best explain food procurement strategies, a critical component of sustainability. In this case, the ABM lends insights into the social evolution of hunter-gatherers in the distant past.

Appendix G. The power of machine learning in uncovering mechanistic processes

The Newton's law of motion can be derived through machine learning based on the mass, charge, geographic positioning information, and so on of all particles in the experiments. Put another way, the machine learning approach ultimately produced a learned mathematical function that exactly "recovers" Newton's formula $F = G\frac{m_1 m_2}{r^2}$ without any previous clue or assumption regarding its form (Figure S3). This suggests AI's major potential to uncover laws or mechanisms in other domains, nourishing an AI-informed ACS and sustainability sciences.

Following 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. If we know the attributes of these agents (users), the amount of renewable water, and the uses of the water, we are likely to derive the possible norms or rules that are hidden but generate such data. Acknowledging the higher difficulty of uncovering laws or rules in Anthropocene systems than in physics or any ACS, we need to strike a balance between seeking the mechanistic processes and its predictive power.

References

1. Steffen, W., Broadgate, W., Deutsch, L., Gaffney, O., & Ludwig, C. (2015). The trajectory of the anthropocene: The great acceleration. *The Anthropocene Review*, *2*(1), 81-98.
2. Turner II, B. L. (2022). *The Anthropocene: 101 Questions and Answers for Understanding Human Impacts on the Global Environment*. New York: Agenda Publishing/Columbia University Press.
3. Costanza, R., McGlade, J., Lovins, H., & Kubiszewski, I. (2014). An Overarching Goal for the UN Sustainable Development Goals.
4. United Nations. (2016). *The sustainable development agenda*. Retrieved from http://www.un.org/sustainabledevelopment/development-agenda/
5. Lade, S. J., Steffen, W., de Vries, W., Carpenter, S. R., Donges, J. F., Gerten, D., … Rockström, J. (2020). Human impacts on planetary boundaries amplified by Earth system interactions. *Nature Sustainability*, *3*(2), 119–128. https://doi.org/10.1038/s41893-019-0454-4
6. The World Commission on Environment and Development. (1987). *Our Common Future*. Oxford/New York: Oxford University Press.
7. Kates, R. W., Clark, W. C., Corell, R., Hall, J. M., Jaeger, C. C., Lowe, I., … Svedin, U. (2001). Sustainability Science. *Science*, *292*(5517), 641–642. https://doi.org/10.1126/science.1059386
8. Council, N. R., Affairs, P. and G., Division, P., & Development, B. on S. (1999). *Our Common Journey: A Transition Toward Sustainability*. National Academies Press.
9. Bettencourt, L. M. A., & Kaur, J. (n.d.). Evolution and structure of sustainability science. *Proceedings of the National Academy of Sciences*, *108*(49), 19540–5. https://doi.org/10.1073/pnas.1102712108
10. Kates, R. W. (2011). What kind of a science is sustainability science? *Proceedings of the National Academy of Sciences*, *108*(49), 19449–19450. https://doi.org/10.1073/pnas.1116097108
11. Clark, W. C., & Harley, A. G. (2020). Sustainability science: Toward a synthesis. *Annual Review of Environment and Resources*, *45*, 331–386.
12. Lubchenco, J. (1998). Entering the Century of the Environment: A New Social Contract for Science. *Science*, *279*(5350), 491–497.
13. Liu, J., Dietz, T., Carpenter, S. R., Alberti, M., Folke, C., Moran, E., … Taylor, W. W. (2007). Complexity of coupled human and natural systems. *Science*, *317*(5844), 1513–1516.
14. Liu, J., Dietz, T., Carpenter, S. R., Folke, C., Alberti, M., Redman, C. L., … Provencher, W. (2007). Coupled human and natural systems. *Ambio*, *36*(8), 639–649.

15. Preiser, R., Biggs, R., De Vos, A., & Folke, C. (2018). Social-ecological systems as complex adaptive systems: organizing principles for advancing research methods and approaches. *Ecology and Society*, *23*(4). Retrieved from https://www.jstor.org/stable/26796889
16. Liu, J., Mooney, H., Hull, V., Davis, S. J., Gaskell, J., Hertel, T., … Li, S. (2015). Systems integration for global sustainability. *Science*, *347*(6225), 1258832. https://doi.org/10.1126/science.1258832
17. Liu, J., Hull, V., Godfray, H. C. J., Tilman, D., Gleick, P., Hoff, H., … Li, S. (2018). Nexus approaches to global sustainable development. *Nature Sustainability*, *1*(9), 466–476. https://doi.org/10.1038/s41893-018-0135-8
18. SDSN Association. (2019). Sustainable Development Solutions Network. Retrieved from http://www.unsdsn.org
19. Harley, A. G., & Clark, W. C. (2020). Sustainability Science: A collaborative community for researchers and teachers. Retrieved from https://www.sustainabilityscience.org/
20. Grimm, V., Revilla, E., Berger, U., Jeltsch, F., Mooij, W. M., Railsback, S. F., … DeAngelis, D. L. (2005). Pattern-oriented modeling of agent-based complex systems: Lessons from ecology. *Science*, *310*(5750), 987–991.
21. Nilsson, N. (2009). *The Quest for Artificial Intelligence: A History of Ideas and Achievements*. New York: Cambridge University Press.
22. Ostrom, E. (2009). A general framework for analyzing sustainability of social-ecological systems. *Science*, *325*(5939), 419–422. https://doi.org/10.1016/j.worlddev.2021.105694
23. Polasky, S., Bryant, B., Hawthorne, P., Johnson, J., Keeler, B., & Pennington, D. (2015). Inclusive wealth as a metric of sustainable development. *Annual Review of Environment and Resources*, *40*(1), 445–466. https://doi.org/10.1146/annurev-environ-101813-013253
24. Janssen, M. A., & Baggio, J. A. (2017). Using agent-based models to compare behavioral theories on experimental data: Application for irrigation games. *Journal of Environmental Psychology*, *52*, 194–203. https://doi.org/10.1016/j.jenvp.2016.04.018
25. Bürgi, M., Östlund, L., & Mladenoff, D. J. (2017). Legacy effects of human land use: ecosystems as time-lagged systems. *Ecosystems*, *20*(1), 94–103. https://doi.org/10.1007/s10021-016-0051-6
26. Holland, J. H. (1992). Complex Adaptive Systems. *Daedalus*, *121*(1), 17–30.
27. Conte, R., & Paolucci, M. (2014). On agent-based modeling and computational social science. *Frontiers in Psychology*. https://doi.org/10.3389/fpsyg.2014.00668
28. Abar, S., Theodoropoulos, G. K., Lemarinier, P., & O'Hare, G. M. P. (2017). Agent Based Modelling and Simulation tools: A review of the state-of-art software. *Computer Science Review*, *24*, 13–33. https://doi.org/10.1016/j.cosrev.2017.03.001
29. Railsback, S. F., & Harvey, B. C. (2020). *Modeling populations of adaptive individuals* (Vol. 63). Princeton University Press.
30. Brown, D. G., & Robinson, D. T. (2006). Effects of heterogeneity in residential preferences on an agent-based model of urban sprawl. *Ecology and Society*, *11*(1), 46.
31. An, L. (2012). Modeling human decisions in coupled human and natural systems: Review of agent-based models. *Ecological Modelling*, *229*, 25–36.
32. Mena, C. F., Walsh, S. J., Frizzelle, B. G., Xiaozheng, Y., & Malanson, G. P. (2011). Land use change on household farms in the Ecuadorian Amazon: Design and implementation of an agent-based model. *Applied Geography*, *31*(1), 210–222. https://doi.org/10.1016/j.apgeog.2010.04.005
33. Sauvageau, G., & Frayret, J.-M. (2015). Waste paper procurement optimization: An agent-based simulation approach. *European Journal of Operational Research*, *242*(3), 987–998. https://doi.org/10.1016/j.ejor.2014.10.035
34. Dou, Y., Yao, G., Herzberger, A., da Silva, R. F. B., Song, Q., Hovis, C., … Liu, J. (2020). Land-Use Changes in Distant Places: Implementation of a Telecoupled Agent-Based Model. *Journal of Artificial Societies and Social Simulation*, *23*(1), 11. https://doi.org/10.18564/jasss.4211
35. Kniveton, D., Smith, C., & Wood, S. (2011). Agent-based model simulations of future changes in migration flows for Burkina Faso. *Global Environmental Change*, *21*, S34–S40. https://doi.org/10.1016/j.gloenvcha.2011.09.006
36. Epstein, J. M. (2014). *Agent_Zero: Toward neurocognitive foundations for generative social science* (Vol. 25). Princeton University Press.
37. An, L. (2022). Complexity. In S. Rey & R. Franklin (Eds.), *Handbook of Spatial Analysis in the Social Sciences*. Northampton, MA: Edward Elgar Publishing.

38. Turner, II, B. L., Meyfroidt, P., Kuemmerle, T., Müller, D., & Chowdhury, R. R. (2020). Framing the search for a theory of land use. *Journal of Land Use Science*, *15*(4), 489–508. https://doi.org/10.1080/1747423X.2020.1811792
39. Taleb, A., Chaussé, A., Dymitrowska, M., Stafiej, J., & Badiali, J. P. (2004). Simulations of Corrosion and Passivation Phenomena: Diffusion Feedback on the Corrosion Rate. *The Journal of Physical Chemistry B*, *108*(3), 952–958. https://doi.org/10.1021/jp035377g
40. Lindsay, A. R., Sanchirico, J. N., Gilliland, T. E., Ambo-Rappe, R., Taylor, J. E., Krueck, N. C., & Mumby, P. J. (2020). Evaluating sustainable development policies in rural coastal economies. *Proceedings of the National Academy of Sciences*, *117*(52), 33170–33176. https://doi.org/10.1073/pnas.2017835117
41. Hornberg, J. J., Bruggeman, F. J., Westerhoff, H. V., & Lankelma, J. (2006). Cancer: A Systems Biology disease. *Biosystems*, *83*(2–3), 81–90. https://doi.org/10.1016/j.biosystems.2005.05.014
42. Chaplain, M., & Anderson, A. (2004). Mathematical Modelling of Tumour-induced Angiogenesis: Network Growth and Structure. In S. T. Rosen, M. Kirsch, & P. McL. Black (Eds.), *Angiogenesis in Brain Tumors* (Vol. 117, pp. 51–75). Boston, MA: Springer US. https://doi.org/10.1007/978-1-4419-8871-3_3
43. Roeder, I., & Loeffler, M. (2002). A novel dynamic model of hematopoietic stem cell organization based on the concept of within-tissue plasticity. *Experimental Hematology*, *30*(8), 853–861. https://doi.org/10.1016/S0301-472X(02)00832-9
44. Folmer, E. O., van der Geest, M., Jansen, E., Olff, H., Michael Anderson, T., Piersma, T., & van Gils, J. A. (2012). Seagrass–Sediment Feedback: An Exploration Using a Non-recursive Structural Equation Model. *Ecosystems*, *15*(8), 1380–1393. https://doi.org/10.1007/s10021-012-9591-6
45. Janssen, M. A., & Ostrom, E. (2006). Empirically based, agent-based models. *Ecology and Society*, *11*(2), 37.
46. Wolfram, S. (2002). *A New Kind of Science*. Champaign, Illinois: Wolfram Media.
47. Axelrod, R. (1997). Advancing the Art of Simulation in the Social Sciences. In R. Conte, R. Hegselmann, & P. Terna (Eds.), *Simulating Social Phenomena* (pp. 21–40). Berlin, Heidelberg: Springer Berlin Heidelberg.
48. Flach, P. A., & Kakas, A. C. (2014). *Abduction and Induction: Essays on their Relation and Integration*.
49. 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. *Annals of the Association of American Geographers*, *95*(1), 54–79.
50. Cumming, G. S. (2008). Complexity Theory for a Sustainable Future. *Columbia University Press*, *New York, NY*.
51. Milner-Gulland, E. J. (2012). Interactions between human behaviour and ecological systems. *Philosophical Transactions of the Royal Society B: Biological Sciences*, *367*(1586), 270–278.
52. An, L., Grimm, V., & Turner II, B. L. (2020). Editorial: Meeting Grand Challenges in Agent-Based Models. *Journal of Artificial Societies and Social Simulation*, *23*(1), 13. https://doi.org/10.18564/jasss.4012
53. National Research Council. (2014). *Advancing Land Change Modeling: Opportunities and Research Requirements*. Washington, DC: The National Academies Press.
54. An, L., Mak, J., Yang, S., Lewison, R., Stow, D., Chen, H. L., … Tsai, Y. H. (2020). Cascading impacts of payments for ecosystem services in complex human-environment systems. *Journal of Artificial Societies and Social Simulation*, *23*(1), 5.
55. An, L., Grimm, V., Sullivan, A., Turner, B. L. I., Malleson, N., Heppenstall, A., … Tang, W. (2021). Challenges, tasks, and opportunities in modeling agent-based complex systems. *Ecological Modelling*, *457*, 109685. https://doi.org/10.1016/j.ecolmodel.2021.109685
56. Vincenot, C. E. (2018). How new concepts become universal scientific approaches: insights from citation network analysis of agent-based complex systems science. *Proceedings of the Royal Society B: Biological Sciences*, *28*(1874), 20172360.
57. Grimm, V., Railsback, S. F., Vincenot, C., Berger, U., Gallagher, C., DeAngelis, D., … Ayllon, D. (2020). The ODD protocol for describing agent-based and other simulation models: A second update to improve clarity, replication, and structural realism. *Journal of Artificial Societies and Social Simulation*, *23*(2). https://doi.org/10.18564/jasss.4259
58. Grimm, V., Revilla, E., Berger, U., Jeltsch, F., Mooij, W. M., Railsback, S. F., … DeAngelis, D. L. (2005). Pattern-oriented modeling of agent-based complex systems: Lessons from ecology. *Science*, *310*(5750), 987–991.

59. Schmidt, B. (2002). The modelling of human behaviour: The PECS reference model. In A. Verbraeck & W. Krug (Eds.), . Presented at the Proceedings 14th European Simulation Symposium, Dresden, Germany: SCS Europe Bvba.
60. An, L., Zvoleff, A., Liu, J., & Axinn, W. (2014). Agent based modeling in coupled human and natural systems (CHANS): Lessons from a comparative analysis. *Annals of Association of American Geographers*, *104*(4), 723–745.
61. Marvuglia, A., Gutiérrez, T. N., Baustert, P., & Benetto, E. (2018). Implementation of Agent-Based Models to support Life Cycle Assessment: A review focusing on agriculture and land use. *AIMS Agriculture and Food*, *3*(4), 535–560. https://doi.org/10.3934/agrfood.2018.4.535
62. Davis, C., Nikolić, I., & Dijkema, G. P. J. (2009). Integration of Life Cycle Assessment Into Agent-Based Modeling. *Journal of Industrial Ecology*, *13*(2), 306–325. https://doi.org/10.1111/j.1530-9290.2009.00122.x
63. DeAngelis, D. L., & Grimm, V. (2014). Individual-based models after four decades. *F1000Prime Rep*, *6*, 39.
64. Gimblett, H. R. (2002). *Integrating Geographic Information Systems and Agent-Based Modeling Techniques for Simulating Social and Ecological Processes*. Oxford, GB; New York, NY, USA: Oxford University Press.
65. von Bertalanffy, L. (1968). *General System Theory: Foundations, Development, Applications*. New York: George Braziller.
66. Axelrod, R. (1997). *The complexity of cooperation: Agent-based models of competition and collaboration*. Princeton, New Jersey: Princeton University Press.
67. Boyd, R., Gintis, H., Bowles, S., & Richerson, P. J. (2003). The evolution of altruistic punishment. *Proceedings of the National Academy of Sciences*, *100*(6), 3531–3535. https://doi.org/10.1073/pnas.0630443100
68. Di Tosto, G., Paolucci, M., & Conte, R. (2007). Altruism among simple and smart vampires. *International Journal of Cooperative Information Systems*, *16*(1), 51–66.
69. Conte, R., & Paolucci, M. (2014). On agent-based modeling and computational social science. *Frontiers in Psychology*, *5*(000668). https://doi.org/10.3389/fpsyg.2014.00668
70. Grimm, V., & Railsback, S. F. (2012). Pattern-oriented modelling: a 'multi-scope' for predictive systems ecology. *Philosophical Transactions of the Royal Society B: Biological Sciences*, *367*(1586), 298–310.
71. Hartig, F., Calabrese, J. M., Reineking, B., Wiegand, T., & Huth, A. (n.d.). Statistical inference for stochastic simulation models--theory and application. *Ecology letters*, *14*(8), 816–827.
72. Bankes, S., Lempert, R., & Popper, S. (2002). Making Computational Social Science Effective: Epistemology, Methodology, and Technology. *Social Science Computer Review*, *20*(4), 377–388. https://doi.org/10.1177/089443902237317
73. Epstein, J. M. (1999). Agent-based computational models and generative social science. *Complexity*, *4*(5), 41–60.
74. Rich, B. R. (1995). *Clarence Leonard (Kelly) Johnson 1910–1990: A Biographical Memoir*. Washington: National Academies Press.
75. CSLI. (2020, May 29). Scientific Research and Big Data. In *Stanford Encyclopedia of Philosophy*. Stanford, CA: The Metaphysics Research Lab, Center for the Study of Language and Information (CSLI), Stanford University. Retrieved from https://plato.stanford.edu/entries/science-big-data/#BigDataKnowInqu
76. Cartwright, N. D. (2019). *Nature, the Artful Modeler: Lectures on Laws, Science, How Nature Arranges the World and How We Can Arrange It Better (The Paul Carus Lectures)*. Chicago, IL: Open Court.
77. Gil, Y., & Selman, B. (2019). A 20-year community roadmap for artificial intelligence research in the US. *arXiv.org*, arXiv:1908.02624.
78. Kipf, T. N., & Welling, M. (2016). Semi-supervised classification with graph convolutional networks. *arXiv:1609.02907 [cs.LG]*.
79. 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. *arXiv:2006.11287 [cs.LG]*. Retrieved from https://arxiv.org/abs/2006.11287
80. Zhang, H., Vorobeychik, Y., Letchford, J., & Lakkaraju, K. (2016). Data-driven agent-based modeling, with application to rooftop solar adoption. *Autonomous Agents and Multi-Agent Systems*, *30*(6), 1023–1049. https://doi.org/10.1007/s10458-016-9326-8
81. Bahdanau, D., Cho, K., & Bengio, Y. (2015). Neural Machine Translation by Jointly Learning to Align and Translate. *CoRR*, *abs/1409.0473*.

82. Nguyen, G., Nguyen, B. M., Tran, D., & Hluchy, L. (2018). A heuristics approach to mine behavioural data logs in mobile malware detection system. *Data & Knowledge Engineering*, *115*, 129–151. https://doi.org/10.1016/j.datak.2018.03.002
83. Chattoe-Brown, E. (2020). Talking Prose All These Years: Agent-Based Modeling as Process-Oriented Analysis. *Canadian Review of Sociology/Revue canadienne de sociologie*, *57*(2), 286–304. https://doi.org/10.1111/cars.12282
84. Hicks, C. C., Levine, A., Agrawal, A., Basurto, X., Breslow, S. J., Carothers, C., … Levin, P. S. (n.d.). Engage key social concepts for sustainability. *Science*, *352*,(6281), 38–40. https://doi.org/10.1126/science.aad4977
85. Carpenter, S. R., Mooney, H. A., Agard, J., Capistrano, D., DeFries, R. S., Díaz, S., … Whyte, A. (2009). Science for managing ecosystem services: Beyond the Millennium Ecosystem Assessment. *Proceedings of the National Academy of Sciences*, *106*(5), 1305–1312. https://doi.org/10.1073/pnas.0808772106
86. Burnham, J. F. (2006). Scopus database: a review. *Biomedical Digital Libraries*. National Library of Medicine. Retrieved from doi: 10.1186/1742-5581-3-1
87. Wu, L., Che Pa, N., Abdullah, R., & Ab. Rahman, W. N. W. (2015). An analysis of knowledge sharing behaviors in requirement engineering through social media. Presented at the 2015 9th Malaysian Software Engineering Conference (MySEC), IEEE. https://doi.org/10.1109/MySEC.2015.7475202
88. De Choudhury, M., Gamon, M., Counts, S., & Horvitz, E. (2013). Predicting depression via social media. *Icwsm*, *13*, 1–10.
89. Rout, J. K., Choo, K.-K. R., Dash, A. K., Bakshi, S., Jena, S. K., & Williams, K. L. (2018). A model for sentiment and emotion analysis of unstructured social media text. *Electronic Commerce Research*, *18*(1), 181–199. https://doi.org/10.1007/s10660-017-9257-8
90. De Choudhury, M., Counts, S., & Horvitz, E. (2013). Predicting postpartum changes in emotion and behavior via social media. In *Proceedings of the SIGCHI conference on human factors in computing systems* (pp. 3267–3276). https://doi.org/10.1145/2470654.2466447
91. Xia, R., & Ding, Z. (2019). Emotion-cause pair extraction: a new task to emotion analysis in texts. *arXiv.org*, arXiv:1906.01267.
92. Gui, L., Xu, R., Wu, D., Lu, Q., & Zhou, Y. (2016). Event-Driven Emotion Cause Extraction with Corpus Construction (pp. 1639–1649). Presented at the Conference on Empirical Methods in Natural Language Processing.
93. Li, X., Song, K., Feng, S., Wang, D., & Zhang, Y. (2018). A co-attention neural network model for emotion cause analysis with emotional context awareness. In *Proceedings of the 2018 Conference on Empirical Methods in Natural Language Processing* (pp. 4752–4757).
94. Zhang, C., Yao, W., Yang, Y., Huang, R., & Mostafavi, A. (2020). Semiautomated social media analytics for sensing societal impacts due to community disruptions during disasters. *Computer-Aided Civil and Infrastructure Engineering*, *n/a*(n/a). https://doi.org/10.1111/mice.12576
95. Goodchild, M. F., & Li, W. (2021). Replication across space and time must be weak in the social and environmental sciences. *Proceedings of the National Academy of Sciences*, *118*(35), e2015759118. https://doi.org/10.1073/pnas.2015759118
96. Li, Y., Zhang, Y., Tiffany, L. A., Chen, R., Cai, M., & Liu, J. (2021). Synthesizing social and environmental sensing to monitor the impact of large-scale infrastructure development. *Environmental Science & Policy*, *124*, 527–540. https://doi.org/10.1016/j.envsci.2021.07.020
97. Janssen, M. A., & Hill, K. (2016). An agent-based model of resource distribution on hunter-gatherer foraging strategies: clumped habitats favor lower mobility, but result in higher foraging returns. In J. A. Barceló & F. D. Castillo (Eds.), *Simulating Prehistoric and Ancient Worlds* (pp. 159–174). Cham: Springer. Retrieved from https://doi.org/10.1007/978-3-319-31481-5_3

---

[i] In ACS 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 [36].

doi:10.20944/preprints202309.1571.v1

[ii] The social sciences have long engaged in abductive reasoning [48] such that ACS science might be seen as a "fourth" way of doing science in the realm, whereas the "third way" is appropriate for the natural sciences.

[iii] 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

[iv] 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".