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Position Paper

Modeling and theorizing with agent-based sustainable development[☆]

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ABSTRACT

Sustainable development is an expression that permeates large areas of knowledge. For it to be meaningful, environmental aspects must be considered as intertwined with economic and social aspects. This is a multidisciplinary effort that is made challenging by the task of synthesizing the many emerging contributions. This has limited theory development where the definition of mechanisms, assumptions, dynamics and the determination of the entities involved are largely left to the reader's imagination. We suggest to engage with the rationale of agent-based modeling to better define the assumptions, mechanisms, and boundaries of sustainable development. For this, the O-part of the widely used ODD protocol for describing agent-based models (ABM) provides a standardized structure, which we here augment to OsDD to specifically take into account sustainability issues. Even without formulating and implementing the full ABM, using OsDD requires to be explicit about the mechanisms, assumptions, dynamics and the entities involved and thereby provides a common language for theory development.

1. Introduction

A key task of environmental sciences is to support achieving the Sustainable Development Goals of the United Nations (2012). While there are many practical and empirical challenges, theoretical and conceptual issues are no less important to address and solve. "Sustainability" and "sustainable development" are umbrella terms (since their beginnings; see World Commission on Environment and Development, 1987) and thereby serve as bridging or boundary concepts. Indeed, this has been useful to policy makers in that they have used this openness to justify a multitude of actions while, at the same time, it makes it difficult to advance the scientific basis that is needed to actually achieve sustainable development. This is because for theory building to take place phenomena need to be precisely defined. "Sustainability" seems to be a particularly difficult concept in this regard as a plethora of definitions exist which may converge on a kernel of congruence, but still deviate sufficiently from one another.

Since sustainability is about what, how, and when human societies exploit natural resources, we need to better understand how both, the natural and socioeconomic systems involved function and, in particular, how they can co-exist and co-evolve as intertwined socio-ecological systems (e.g., Folke et al., 2005; Partelow, 2018; Biggs et al., 2021; Purvis et al., 2019). To this extent, theories and theory development play a critical role. We here refer to both ways in which the term "theory" is widely used: *heuristic* theory – an assumption or hypothesis of how a certain phenomenon could be explained, which is how "theory" is used in colloquial language; and *scientific* theory – an explanation of a phenomenon that is supported by a vast body of evidence. Sustainability science needs more and better of the latter type – i.e. scientific theory – so that actions and policies designed to foster sustainable development will be more likely to have their desired effects.

Heuristic theories formulated in sustainability science are usually too ambiguous to be tested and thereby developed towards scientific theories (Troullaki et al., 2021). These heuristic theories are expressed verbally, allowing different conceptualization of the same (or similar) expression(s) as well as a diversity of expressions to indicate the same concept. In some cases, they are expressed under the label of a "framework" and characterized as "a set of assumptions, concepts, values and practices that constitute the way of viewing the specific

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reality" (Binder et al., 2013, p.2). They remain vague and subject to different interpretations, especially when they take a social-ecological perspective on sustainability (Binder et al., 2013). Such conditions of a field are barriers to conceptual clarity. Nonetheless, conceptual clarity is a prerequisite for the advancement of research generally, and theory development specifically.

Moreover, because it is too easy to formulate just another theory, there are too many theories and they are disconnected from each other mainly because they belong to different disciplines, a key feature of sustainability science (e.g., Robert et al., 2005).

Agent-based modeling (ABM) could help improve this shortcoming because it forces scientists to make their claims explicit. In this way, the conceptual model of the world, system, or phenomena that is the subject of the simulation has to take a programmable form, something which can be classified as a flexible form of formalization.[1] It is this flexibility that makes ABM the most likely approach to connect between different disciplines.

Ideally, each new heuristic theory that is suggested would be implemented as ABM, linked, if necessary, with other model types. Although this thought is intriguing, it is unlikely to be feasible and could also slow down, or even hinder, free and fresh thinking that lead to new theories. Still, even if just the structure and processes of a model that would implement the theory is to be specified in a certain format, including specific descriptions of the key processes of the theory, the current ambiguity and proliferation of heuristic theory could be considerably reduced. We consider this a compromise, a *minimum requirement* or, in other words, a necessary step to be met by those who wish to develop sustainability theory. We are not suggesting that scholars stop there. Of course, moving further in the development of agent-based models would contribute to an active assessment of theory (more specific information on ABM can be found in Grimm and Railsback, 2013; Edmonds and Meyer, 2017; Gilbert, 2008; Secchi, 2022).

Using an example from psychology, when trying to better understand the dynamics of learning a new language by immigrants, Caldwell-Harris (2019) developed an agent-based model that allowed, and forced, her to formulate theories explicitly and unequivocally. The format she used was the *Overview, Design concepts and Details* (ODD) protocol, a now widely used standard format for describing ABM (Grimm et al., 2006, 2020b, see Table 1). Even though she did not implement her model, she summarized the benefits of formulating an agent-based model using the ODD protocol: "The ODD protocol provided an organizing framework in which many details were worked out. ... Answering the ODD questions required identifying outcome variables (frequency of use and fluency in the two languages), basic entities (representing individuals, families, neighborhood, global environment), rules for initiating and continuing conversation, and rules for agents to move to new locations" (p.120).

The 'O' (or *Overview*) part of the ODD protocol would not only force us to be more explicit about the details of heuristic theories, it would also help speaking a common language by using the ODD terms to describe our models and theories. The lack of a common understanding of terms and measures to quantify phenomena is a well-known major impediment to a successful development of theory and applications within and between any discipline (see the review by Hill et al., 2012). Over the years, there have been many attempts to create a common frame for sustainability. One such attempt relates to the use of systems thinking in sustainability management (e.g., Williams et al., 2017), considered as a way to bridge concepts across disciplinary domains. Another approach is devoted to the development of a "proto-theory" in sustainability management research (Starik and Kanashiro, 2013) that, again, is aimed at emphasizing that complexity, wickedness, multi-scale and multi-level interactions cannot be successfully considered by mono-disciplinary research. Yet another study aimed at supporting multi-disciplinary sustainability research focuses on computational methods (Chatterjee and Rao, 2020). All these and other studies are noticeable attempts although they do not describe a process directed towards theory development. We claim that the modified version of the ODD protocol presented here (called OsDD) integrates and complements existing attempts by providing guidance on some of the most relevant aspects to consider in developing theory for sustainability research.

We therefore believe that we should be able to draw on the different branches of sustainability science – i.e. economic, social, and environmental – to establish a connection through ABM. In so doing, we take inspiration from and work on a modified version of the *Overview* part of the updated ODD protocol for ABM (Grimm et al., 2020b). In the following, we first describe the current range of the most important theoretical perspectives on sustainability, followed by a discussion of the most relevant issues related to them. We then describe how ABM and ODD can be used to formalize the description of heuristic theories addressing sustainability and present a roadmap as a guide to researchers' perusal. While the approach we are suggesting will not resolve all challenges related to defining and actually promoting sustainability and sustainable development, it has, as it is simple and straightforward, the potential to advance the field.

2. Theoretical perspectives on sustainability

The exercise of isolating theories of sustainability is challenging. This is a direct result of the dispersed and wide nature of the field as well as of the different meanings attached to what *sustainability* actually entails. One way to explore theories is to study the different conceptualizations present in the literature. They clearly indicate a diverse understanding of the topic. This section is a selection of those conceptualizations that make diversity more apparent.

2.1. The basics

The original definition of sustainable development is vague enough to understand the conceptual, theoretical, and construct variety that came after it. The most widely accredited source for a first definition is the Brundtland Report. It states that

> "humanity has the ability to make development sustainable to ensure that it meets the needs of the present without compromising the ability of future generations to meet their own needs" (World Commission on Environment and Development, 1987, par. 27).

Not only this definition makes explicit reference to demands that are to be met in order to satisfy the current necessities of the human population, but it also refers to a demand–supply *equilibrium* to be met in the future. Whether these "needs" refer solely to humans as active in the economic market or, more broadly, as citizens in their respective societies is specified in other parts of the report. And it is clear that the document leans towards the latter, i.e. the focus is on citizens embedded in their societies. At the same time, the conceptualization of "needs" is vague enough to suggest that most of them are satisfied through a market mechanism, implying production and consumption over the exchange of monetary means. These "needs" are, in broad terms, to be intended as the necessary means humans have to survive – i.e. they are *basic needs* (World Commission on Environment and Development, 1987). The above can be read as the tendency to frame sustainability as the search for a solution to a practical problem (Norton, 2010; Burger and Christen, 2011). This resonates with *economic* approaches to available resources, since they are usually concerned with objectives and scarce resources (Marshall, 2009).

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[1] Computational models are based on formal logic that is coded and programmed. Logic is part of mathematics and, as such, computational modeling is effectively based on a formal language. We thank one of our reviewers for inviting us to reflect more deeply on this and debunk the view that computational programming is, in the eye of more traditional modelers, a less noble form of formalization.

2.2. Intergenerational interactions

The perspective described above has, over the years, brought about a varied multi-dimensional approach to sustainable development. The necessary means to survive for generations to come is inevitably bound to today's use of world resources. By operating more consciously (responsibly) on the earth's resources we may be able to guarantee a future for forthcoming generations. This inter-generational equity was only partially present in theories and models of *economic* development before the emergence of concepts emphasizing the notion of *sustainable* development. This underscores the importance of *time* as an essential dimension in the sustainability discourse and the dynamics arising from it. By the use of the expression "future generations" this continuity is made discrete, perhaps in an opening to measurement and assessment of progress (Forouli et al., 2020).

In particular, the aspect of inter-generational equity merits further attention, especially when sentiments around sustainability become more visible. In fact, not only the concept casts a forward-looking perspective on socio-economic systems, but the way in which it is perceived varies significantly from generation to generation. Several studies have shown that younger people – e.g., the so-called Generation Z (b.1995–2009) and Generation Y or Millennials (b.1978–1994) – are more likely to prefer an employer that actively promotes sustainability (Greening and Turban, 2000; Gully et al., 2013; Rupp et al., 2013), show higher levels of responsible consumer behavior (e.g., Kamenidou et al., 2019; Su et al., 2019) and are, in general, more socially conscious (Klimkiewicz and Oltra, 2017; Yamane and Kaneko, 2021). This trend is expected to be even more salient among Generation Alpha (b.2010–2024) who will start to enter the workforce within the next decade. It is also projected that future generations (such as Alpha) can be up to seven times more affected by climate change; emphasizing the growing importance for the aforementioned inter-generational solidarity (Thiery et al., 2021). Under this lens, sustainability is a psychological and cognitive perspective that drives individual and group behavior. While research on generational differences has seen its critics, we interpret the evidence cited as offering partial support for the claim on these differences.

2.3. The socio-economics of sustainability

A second aspect of the multi-dimensional approach appears when one reflects on the implications of "needs" satisfaction (Purvis et al., 2019). As mentioned above, this is mainly referred to an economy where goods and services are exchanged (Meadows et al., 1972). At the same time, these goods and services are affected by and affect the environment, intended as the varied natural ecosystems that surround human beings. Here a social (human) dimension is intertwined with another social (economic) dimension to influence (and be influenced by) an ecological/environmental dimension. The consumption of an apple wrapped up in plastic implies that an organization must have produced it, sold it to a supermarket that priced it and then sold it to a consumer. To preserve its freshness, plastic has been used, and this plastic had to be produced by another organization. Not only consuming products that come directly from a natural ecosystem affects our "needs" but they affect nature as transportation and plastic production are traditionally linked to emissions that have negative effects on nature. The cycle does not stop here since consumers also play a role when they make a purchase and subsequent waste disposal decisions. When including this latter aspect, one is clearly referring to what is generally called *circular economy*. This is the consideration that every aspect of our socio-economic behavior has implications on the system unless it is appropriately taken care of. Hence, the need to close the loop and make sure that products are not simply disposed after they have been used, but have the chance to re-enter production (Winans et al., 2017; Nikolaou and Tsagarakis, 2021).

In other words, the three basic dimensions that have traditionally been connected to the concept of "sustainability" and "sustainable development" are the *economic*, the *social*, and the *environmental*. These three aspects considered together are widely known as the *triple bottom line* (Purvis et al., 2019), that counts as another conceptual perspective on the topic (Hopkins, 2016). Although the two expressions of "sustainability" and "sustainable development" are considered synonym by the majority of scholars, the latter has economic overtones while the former is more in line with environmental perspectives (Bolis et al., 2014). A historical account of the triple bottom line by Purvis et al. (2019) provides several examples of the way in which the concepts are used to stress at times one aspect or another.

The above calls for a multi-disciplinary approach that has been labeled *sustainability science* (e.g., Troullaki et al., 2021; Kajikawa et al., 2014) to indicate the unprecedented need to bring diverse perspectives together if social, economic, and environmental problems are to be solved. A general idea of the range covered by this dimension is given by the simple read of the 17 United Nations Sustainable Development Goals (https://sdgs.un.org/goals). These range from the global challenge to end poverty (SDG 1) to sustainable industrialization (SDG 9), from ensuring quality education to everyone (SDG 4) to water conservation (SDG 14). The goals are not grouped into coherent macro areas but it is relatively easy to read between the lines and find that some belong to economic/business research areas, some others to broader social sciences perspectives while there are some that are clearly bound to environmental sustainability (an in-depth presentation of the SDGs is in Hoek, 2018).

2.4. Sustainability assessment

Yet another way to conceptualize sustainability relates to a line of enquiry that goes under the label of *sustainability assessment* (SA) and, within it, that of Life Cycle (Sustainability) Assessment (LC(S)A; Troullaki et al., 2021). This latter "can be used to study the environmental impact of either a product or a function the product is designed to perform. LCA is commonly referred to as a 'cradle-to-grave' analysis" (Glavič and Lukman, 2007, p.1880). In this respect, the idea of sustainability coincides with that of its tracking or with the way in which it is measured. Better sustainable practices are those that minimize the overall LCA impact of a product or function. From a different but related perspective, "assessment" is sometimes framed as "accountability" and it relates to how organizations measure and report sustainability actions. This stream of research overlaps with that of corporate accountability, auditing and reporting (Gray, 2001) and it has been indicated as one of the main perspectives in the social responsibility of businesses (Secchi, 2007). In recent years, the Global Reporting Initiative (GRI; http://www.globalreporting.org/) is by far the most widely used standard for sustainability reporting.

A different perspective altogether is that of those who decided to focus on a single aspect of sustainability, leaving the other two on a side. These approaches go under a series of names that identify the specific discipline to which they refer to. Examples of these streams are, *circular economy*, *bioeconomy*, *social responsibility*, *ecological footprint*. Table 1 presents an overview of different interpretations that can be attributed to sustainability from the perspective of each of its "branches" – i.e. economic, social, and environmental. These are "emphases"' and reflect a general study frame that is exemplified by the "keywords' in the next column, as to indicate streams that seem to be guided by the statement in the column "emphasis"' or by parts of it. The last column on the right offers a (by no means comprehensive) selection of references where these claims are practiced.

3. The matter of concern

There are a series of concerns that surround the generic conceptualizations of sustainability that many scholars use. They can be divided in two blocks, one pertaining to *interpretation* while the other to *theoretical advancements*.

Table 1

Different interpretations of sustainability.

Areas	Emphasis	Keywords	Reference
Economic	The emphasis is on ways to balance economic growth paths with the preservation of human existence on the planet.	Green economy, bioeconomy, circular economy	Meadows et al. (1972), Nikolaou and Tsagarakis (2021) and Winans et al. (2017)
Social	The physical and psychological well-being of humanity's future depends on the mindful (sustainable) management of natural and economic resources.	Sustainable tourism, social responsibility	Bolis et al. (2014), Higgins-Desbiolles (2020), Frey (2021), Morganti and De Giovanni (2022) and Secchi (2007)
Environmental	The focus is on the preservation of natural resources when human activity is present.	Ecological footprint, bioenergy, sustainable agriculture	Kajikawa et al. (2014), Finnveden et al. (2009) and Pretty (2008)

3.1. Divergent interpretations

One of the main aspects that the short overview above brings forth is that the concept of sustainability is broad. This is not necessarily a problem per se – the social sciences have had some success working with inherently vague concepts – but it can become a problem when consistency of interpretation is challenged. We argue that scholars approaching a concept from the same discipline typically interpret it from the perspective of a common understanding. In other words, language indicating shared understandings of concepts is the basis for such scholarly work. The backbone of their knowledge is more or less consistent: they use similar underpinning assumptions and theories. This is problematic because it only allows for a vague conceptualization to maintain core characteristics of shared meaning. There are many examples of loosely formalized theories that maintain their core characteristics within the same and within closely related fields – e.g., sensemaking (Weick, 1993), self-efficacy (Bandura, 1997), competitive advantage (Porter, 1985). When this *interpretive milieu* falls – that is when access to the concept happens by scholars from different disciplines – there is a possible lack of consistency, changes in meanings, and slight differences in understandings for a concept that is kept too broad. Consequently there is a risk is that the same concept matures into different (possibly divergent) interpretations depending on the field in which it has its origins. For example, this is the case of *stakeholder theory*, a concept developed by strategic management scholars in the Eighties (Freeman, 1984) and meant to challenge the classic shareholder-centered perspective of the firm. When transferred to a wider sustainability context, the concept has been watered down to signify those who have an interest in a given phenomenon. In other words, it has lost the organization as its main point of reference, its original theorization, its reference to shareholders, and the related strategic implications for the management of companies.

In the case of sustainability there is an additional challenge related to the fact that its conceptualization needs to adapt to the changing circumstances of human life. For example, on the one hand, a balance of needs between generations can be agreed and defined specifically. On the other hand, these inter-generational needs change over time and new ones add to or substitute old ones. The COVID-19 pandemic has induced some to reflect on the fact that we must defeat the virus right now while also allowing future generations to be more proactive in fighting similar challenges. Hence, pandemic management has entered the domain of sustainability-related topics (Brousselle et al., 2020; O'Flynn, 2021).

The above points at the need for the conceptualization of sustainability to be firm, yet inclusive and flexible. This posits an incredible challenge to scholars because one may well ask what are then the criteria to make a decision on what to include or exclude from the sustainability domain. Put differently, there is a risk that the concept would stretch so much that it lacks scientific tractability. Similar examples have been found in the conceptualization of hubris (Zeitoun et al., 2019) and the so-called "Green Human Resource Management" (e.g., Wen et al., 2022), where extensions of existing conceptualizations generate ambiguity rather than clarity.

3.2. Theoretical advancements

The vacuity surrounding the concept of sustainable development has been denounced many times (Troullaki et al., 2021; Burger and Christen, 2011). Not only the concept is currently used by scholars with meanings that maintain their domain specificity (see Kajikawa et al., 2014; Bolis et al., 2014), but also those who use versions of multi-disciplinary approaches (e.g., Baldos et al., 2020) seem to lack interest in defining it more rigorously. This lack of a feedback loop that brings new knowledge back to discuss the nature and meaning of sustainability is concerning because it does not help the research area move forward.

Of course, one may argue that sustainability is an umbrella term, something that is used more as a paradigmatic framework rather than a proper theory. This is probably accurate, its proponents have never called it a theory. Nor those who use it call it a theory. However, a paradigm cannot be used as a static immutable reference where various theories find place and use. The paradigm should allow for theories to be developed under its frames. Has this happened with sustainability? This is very difficult to assess. As far as our knowledge is concerned, it is mainly the opposite that has happened. That is, existing theories use a sustainability frame to gain broader applicability. This is the case of stakeholder theory (Freeman, 1984; Freeman et al., 2003) that is very often used together with sustainability (Glavič and Lukman, 2007) to help with the assessment of the various actors involved. The same barrier to theory development fostered by umbrella terms occurred in ecology and socio-ecological research, where the terms "stability" (Grimm and Wissel, 1997) and "resilience" (Brand and Jax, 2007) are often used to burnish the interpretation of empirical or theoretical studies.

4. An agent-based approach to sustainability

The sections above serve the purpose of highlighting that sustainability has remained a broad concept (a paradigm, we have suggested) that does little to inform (and be informed by) the theories that it employs. This is due to a very difficult relation between applications coming from a variety of fields and the paradigm itself. The changing nature of the "needs" (World Commission on Environment and Development, 1987) brings additional challenges.

To better integrate the different disciplines, concepts and languages involved, we suggest to build on the unifying potential of agent-based modeling (ABM). ABM is a particular form of computational simulation where the focus is on the "agents" – i.e. the many autonomous and heterogeneous entities that are used to develop the model (Grimm et al., 2005). This implies that any ABM should consider and discuss what is meant by "agency". ABM should also include mechanisms that define interactions between agents, their evolution, and co-evolution with the environment (Gilbert, 2008; Secchi, 2022). Another relevant feature of this class of models is that they allow for stochasticity to be added with limited constraints in any of their elements. The mix of these aspects allows ABM to be particularly effective in representing complex systems (Edmonds and Meyer, 2017; Grimm et al., 2005).

In this section, we explain how a widespread use of ABM may offer support to sustainability-based theoretical developments. In so doing, we are focusing on three concerns, namely the role of time, disciplinary boundaries, and uncertainty of definitions.

Before we move to discuss these concerns, we should add some epistemological considerations, specifically on the type of knowledge that is conveyed to sustainability by the use of ABM. On the one hand, ABM can be considered to lean on a *process* (Miller, 2015) or on a *variance* approach (Van de Ven and Poole, 2005). The first emphasizes how a system's change is necessarily tied to a variety of phenomena, elements, and conditions that manifest over time, while the second is concerned with the assessment and measurement of variations due to a selected number of initial conditions. For the case of theory development in sustainability research, we argue that both approaches are relevant for ABM.

The three concerns below substantiate some of the reasons why this epistemological claim is valid. While ABM is bound to processes, in the sense that the way in which it evolves is based on rules (or *mechanisms*) that structure co-evolution over time (as in a process approach), it also defines settings – both agent characteristics and related parameters – that can be studied in relation to one or more outcome variables (as in a variance approach). Hence, we are not convinced that either one (i.e variance approach) or the other (i.e. process approach) is the appropriate way to categorize ABM, since there are aspects in ABM that converge towards a process and others that are aligned with a variance approach (Van de Ven and Poole, 2005; Miller, 2015). Instead it is our view that ABM should be classified as a "bridging" approach that does not fit neatly into the distinction between variance and process studies. This is due to the fact that on the one hand ABMs rely on emergence and are able to deal with nonlinear effects and time delays (i.e. process approach; see also, e.g., Davis et al., 2007) and thus are suited for theory development. On the other hand they generate data that then can be subjected to more traditional statistical analysis (i.e. variance approach). Starting from this vantage point, it becomes important that sustainability researchers clarify which part of their theoretical development leans towards a process or a variance approach and we outline these points in the subsequent sections.

4.1. Time-related meanings

In the preceding sections we argued that the time dimension appears to be a fundamental component sustainability discussions. This component can be framed socially, in terms of the balance between present and future generations' needs (World Commission on Environment and Development, 1987), or it can be framed in terms of the opportunities for economic growth (Meadows et al., 1972). Or, again, it can be framed in terms of the management and preservation of natural resources (Bolis et al., 2014).

Not only are there multiple time-related trade-offs between generations, but they change and evolve depending on how society, the economy, and the severity of environmental issues evolve. Consequently, this points at the need to consider these as nested (wicked) problems.

ABM has the flexibility to show how trade-offs may work over time. This is usually executed by considering slow and fast timescales at once. In fact, as some have argued (Neumann and Cowley, 2016) ABM allow researchers to study the way in which macro-structural elements such as norms, values, and cultures affect and are affected by the actual behavior of agents. The former typically develop on slow timescales while the latter are framed on fast timescales (see Secchi, 2022a).

The latter affects the former and vice versa, passing through various configurations of the "middle" or, better, *meso* domain (Secchi and Cowley, 2021; Secchi et al., 2022). More generally, any attempt to manage a social-ecological system towards a certain goal, for example resilience, has to consider short, intermediate, and long time scales, which are linked to different decision contexts and levels of perceived urgency to act. Weise et al. (2020) refer to this a "resilience trinity" and claim that management has to reconcile all three time scales to be successful in terms of safeguarding or restoring resilience. The same holds for sustainability.

For example, in an inspiring agent-based model of fisheries (Madsen et al., 2021) show that sustainable fishing depends heavily on a mix of policy (e.g., quotas and protected areas) and decision making heuristics (e.g., from strictly rational to pseudo-random). Re-written using the jargon above, these authors show that the slow timescales affect fast timescales and, depending on goal efficacy, the latter could eventually change the former.

Another example is that of Bazzana et al. (2020) where the water-related needs of a community are contrasted with the energy generated by the construction of a dam. This article tackles two equally important sustainability objectives: (a) protecting a fundamental access to resources of a community and (b) being able to produce renewable energy. In this case, the latter may hinder the former. Both objectives are set to be effective in the long term but the actions and the decisions are made here-and-now, in the fast timescale. The model of this paper helps reflect on these issues and provides good grounds for institutional decision makers in developing countries.

It should be apparent by now that the dichotomy between short and long timescales is not something secondary for sustainability research. Quite the contrary, it is essential to its core message. In fact, sustainability is set to achieve results that are stable and capable of changing the way in which human action affects the environment and all of its resources. This means that sustainability research always has the tendency to understand its effects on slow timescales. At the same time, operations are only applicable and analyzable on fast timescales (Weise et al., 2020).

4.2. Across disciplinary boundaries

Calls to integrate sustainability disciplines under one umbrella have multiplied in recent years among scientists (e.g., Lang et al., 2012). Since each discipline has its own terminology, concepts, and culture, a necessary condition for integration is a common language. Mathematics, in particular calculus, provides such a language for physics-related disciplines. However, mathematical models are not flexible enough to adequately take into account not only environmental, but also ecological and social factors, as required for sustainability research. Agent-based models can take into account these three different types of factors, in particular the agency of organisms, humans, and institutions. Moreover, agent-based models are implemented as computer programs, not as a set of equations. The logic-bound nature of programming languages makes it relatively easy to combine and interpret independent of the disciplinary background of the scholar.

Still, designs and descriptions of ABM differed a lot between disciplines, which led to the development of the ODD protocol (see introduction). And indeed it has been shown that ODD has already contributed to integrating disciplines. In a bibliometric analysis, Vincenot (2018) shows that the literature using the term "agent-based", as models are called in social sciences, and "individual-based", as they are usually called in ecology, is increasingly overlapping in terms of citing the same references. Vincenot (2018) showed that ODD played an important role in this process and suggested that this is due to ODD providing a common language across disciplines.

The argument above on the flexibility of ABM to work across disciplines resembles old claims made by systems theorists who advocated that, since most phenomena in science can be offered a system-like representation, their mathematical properties could be transferred across disciplines. This would mean that systemic properties in one field could be applicable to other fields. The structure took priority and prevalence over the context of application (Neumann and Secchi, 2016). Agent-based modeling shares the knowledge-expanding aim of this view, but it approaches it differently.

First of all, the language which is used by ABM is more approachable and less rigid than the one of systems theory. The former uses computational means to study phenomena while the latter used mathematics, especially differential equations (e.g., Beer, 1965; Forrester, 1980). While the interpretation of a coefficient in an equation can be particularly specific and require skills and knowledge that are specific to that domain of mathematics, computational work is usually more flexible. Not only computational notations are typically expressed in a way such that specific knowledge may not be necessary, but their working mechanics can be inferred by observing how the model functions as a whole. Computational work is, contrary to equation-based modeling, a system that works *through doing* (Secchi, 2022). This means that, in order for ABM to make sense, it is necessary that the researcher manipulates the working elements of the model (Secchi, 2022, Chapter 2) to develop an understanding of the simulation model and, at the same time, to make the simulation work.

By emphasizing the working elements of ABM, it is clear that the 'transfer' is not based solely on the structural elements of a system. Instead, the researcher is committed to work on the mechanisms that may or may not apply across disciplines. The mechanisms[2] (or working elements) enable structural properties but they cannot be considered such. This is for two reasons. One is that ABM generates complex systems and slight changes in one component may trigger dramatic shifts in the outcome variable (Miller and Page, 2007; Epstein, 1999). The other is that the meaning of one mechanism can be different when transferred to another model, in the context of another discipline.

The main claim of this subsection is that ABM are powerful tools to enhance cross-disciplinary knowledge transfer.

4.3. Data issues

One of the strengths of ABM is that the requirement for input data varies with the simulation objectives. This means that, in theory, an agent-based simulation can be created in absence of empirical data, by using conjectures, arguments, and previous research. This is the case of Secchi and Herath (2021) where the simulation is built on assumptions (derived from extant literature) to understand what is the likelihood that a particular phenomenon would manifest itself. The authors take the actual case of a neighborhood in Copenhagen and explore whether residential segregation would generate aggregation of people with similar "unorthodox" societal values. Sustainability is here considered in its socio-economic dimensions only but still consistent with common definitions (e.g., United Nations' SDG). What is important to notice here is that the model in Secchi and Herath (2021) does not use any empirical data, but only works on 'as-if' scenarios. Given policy makers use assumptions that are sometimes not grounded on facts, sustainability research needs to be able to work on counterfactual assumptions. ABM is an approach that makes this relatively easy, compared to other research instruments.

Simultaneously, ABM allows for the most granular and detailed description of the observed phenomenon. In fact, when data is available, researchers may want to use as much as possible to define their agents, environment, mechanisms (see Herath et al., 2017). This is a change in modeling perspectives that some (Edmonds and Moss, 2005) have called KIDS – 'Keep It Descriptive, Stupid!' – in opposition to the classic KISS – 'Keep It Simple, Stupid!' Some areas of sustainability may be data heavy and allow to regulate a model on to existing or collected evidence. This is the case of, for example, models that attempt to predict production levels of renewable energy sources (as in Mahmood et al., 2020).

In most cases, the line is somewhat in-between the two cases outlined above – i.e. no data at all, and full data details. This is especially the case in sustainability research, where some data is available, mainly from the natural/engineering part of a study, and more limited or incomplete data sources are more likely to appear in the socio-economic part. When this is the case, researchers try to supplement their research with additional primary qualitative or quantitative sources. In a study of the potato late blight control in the Netherlands, Pacilly et al. (2019) indicate that their simulation can be referred to as "midrange" (p.356) since it does not fall in to any two of the types above. Their focus is on understanding how decisions compared in relation to the evolution of the disease. Yet, due to data scarcity, the authors used semi-structured interviews with farmers. As such, an ABM approach provides policy makers a computational testbed to explore abductive reasoning. Where one could begin with an incomplete set of observations and proceed to exploring likely possible explanations through simulating a varying range of 'as if', 'what if' scenarios and trajectories. This differentiates an ABM approach to most other approaches where such, robust abductive exploration is not possible.

5. A roadmap for agent-based sustainable development

This section is dedicated to a practical hands-on guide to build agent-based models that would help support sustainability-focused theories. As anticipated in the introduction, we use a modified version of the *Overview* part of the ODD protocol (Grimm et al., 2020b) as an operational guide. The ODD protocol was originally introduced to standardize the documentation of agent-based simulation models (Grimm et al., 2006). It then turned out that it can also be used to conceptualize, design, and specifically formulate an ABM even before it has been implemented. To achieve this aim, the seven ODD elements are used as a checklist and guide.

ODD is comprised of seven elements which are grouped into three blocks: *Overview*, which provides an overview of the model's purpose and patterns, entities, state variables and scales, and processes. For the latter, no details are included, only the list of processes, such as trading, growing crops, changing land use, or, on the ecological side, growth, reproduction or foraging. This 'O' helps to easily navigate even in long descriptions of complex models, and it allows to quickly grasp what the model is and does, which also facilitates comparison to other models. The second block, *Design concepts*, comprises 10 important concepts that explicitly should be addressed and used in the design of an ABM, for example interaction and stochasticity. The third block, *Details*, includes a full description of the models initialization, input data representing external drivers, and sub-models which implement the process listed in the Overview.

In its initial formulation, it was mainly aimed at ecology scholars (Grimm et al., 2006), but it has been extended to social scientists (Polhill, 2010), and updated again recently (Grimm et al., 2020b). A full description of ODD and its rationale, and detailed guide for its use, including many examples and dos and don'ts, is provided, open access, in Grimm et al. (2020b).

Here we are suggesting to use a slightly modified version of the O-part of ODD to facilitate theory development. This will and should be complemented by formulating, developing and testing full models. But since model development is time consuming, it would take too long to have critical mass of agent-based models addressing a certain theoretical domain. Conceptual modeling by itself can already, as we saw in the example from psychology cited in the Introduction, pave the way for theory development by overcoming the ambiguity of unstructured verbal theory formulations. In other words, explicitly inviting to reflect

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[2] We are not claiming that the mechanisms are sufficient to generate the outcomes of a model or should be considered in isolation (León-Medina, 2017), that they are one of several accounts of causation (Manzo, 2022), yet they maintain a relevant role in the perspective of ABM for sustainability theory development.

on these elements ex ante may help understand and better frame the various components of sustainability modeling.

The *Overview* part of ODD is made of three parts: 1. Purpose and patterns, 2. Entities, state variables and scales, and 3. Process overview and scheduling. We are augmenting these with a few elements, and refer to the modified Overview part, and hence the entire ODD, as OsDD, the "s" standing for "sustainability". Similar modifications of ODD for specific purposes exist, such as ODD+D (Müller et al., 2013) for describing models which include human decision making, and M-ODD (Savić et al., 2022) for models describing mobile ad hoc networks. Table 2 provides a summary of the points presented in this section.

5.1. Purpose, patterns, and propositions

When describing the *purpose* of a model, scientists should clearly state both, the overall purpose of the model and the general and specific research questions asked. Both of these determine to a large degree the design of the model, without knowing them it would be impossible to assess whether a model's design makes sense. Stating purpose and questions also defines the scope of the model, because for other questions and purposes, even about the same system, different design might be needed. Using a model outside its scope, in particular its purpose, is common practice in ecology and can make theory development impossible.

Recently, some have suggested a general typology of modeling purposes (Edmonds et al., 2019), ranging from explanation and description to theoretical exploration, illustration, analogy, and social interaction, and prediction. Grimm et al. (2020a) boiled this down to three main categories: demonstration, understanding, and prediction. Thus, when the O-part of OsDD is specified for a certain theory addressing sustainability issues, it would be clearly communicated whether the theory is more on the heuristic or on the scientific side.

In sustainability research, a reflection on the purpose of a model is particularly important because of the nature of this field of study. In fact, a clarification of the aim towards which the model is oriented serves as an indication of its breadth. An example could be a model that is concerned with connecting consumer behavior with greenhouse gas emissions, depending on alternative normative scenarios (Bravo et al., 2013). When having an integrative sustainability approach in mind, one could immediately check whether (a) the different aspects of sustainability are considered (i.e. environmental, social, economic) and whether (b) the approach taken is such that knowledge from multiple disciplines is involved. In this case, a check of (a) is very much apparent while a check of (b) would depend on how the purpose is specified through propositions (see below). In principle, one could either use economics to explore the purpose or need integration with food science, behavioral science, and engineering. In light of the above, the second choice would be preferable, hence reflected in the purpose as much as possible (see Table 2).

The second element under ODD's O-part is *patterns* (see Table 2). These are the patterns, stylized facts, observations, or data that will be used to claim that the model is realistic enough for its purpose, i.e. the model should be able to reproduce these pattern. This element is included because in particular for predictive models, the patterns or data available for validating the model often strongly influence the model's structure ("pattern-oriented modeling;" Grimm et al., 2005; Grimm and Railsback, 2012). However, for the conceptual modeling that we are advocating here, the overall model purpose will be more on the demonstration and understanding side. Still, it would be important to know, from a theory that proposes to explain phenomena which are relevant for sustainability, what kind of observations from the real world they are supposed to explain or, more generally, which observations would be used to claim that the model is correct.

ODD refers to patterns, not data, because "data" broadly refers to specific numbers, while "patterns" includes broader generalities. For example a certain variable stays within certain ranges, or that under condition A, agents show certain kinds of behavior more often then others, while under condition B this is not the case. Grimm et al. (2020b) call such patterns "weak" patterns, as they are sometimes reproduced to be a set of alternative models, but, as it has been shown in ecology (and also in economics) trying to make a model reproduce several weak patterns simultaneously provides a powerful means to reduce uncertainty in model structure and parameters. Gallagher et al. (2021) reviewed the patterns used for "pattern-oriented modeling" in ecology, a similar review in sustainability science would be worthwhile.

Patterns are intended as a way to easily assess whether the purpose has reached its aims or not. Patterns can be defined qualitatively but, at the same time, they shall be testable (Grimm et al., 2020b, S1: ODD Guidance and Checklists). From a cross-disciplinary perspective this aspect of the Overview raises a few concerns that need to be clarified. In fact, the expression 'qualitative testable patterns' is a contradiction in terms from the perspective of a social scientist. Qualitative research design in the social sciences is not intended to be testable but is aimed at describing and understanding phenomena, mainly asking *why* questions and being unconcerned about precision of mechanisms or generalization of findings. Moreover, a pattern in ABM almost always implies temporality – i.e. where the regularity (or repetition) of a phenomenon is present. As such, while some qualitative accounts might capture this time-related aspect, it is not consistently seen in such designs especially in a testable form. Therefore, when calling for ways in which disciplines may be considered together – such as in sustainability research – there is a need to make sure that the way in which we frame the model is compatible across them. The second issue with patterns is that the result of a model may not be expressed in this form. For example, a model that simulates diffusion of bio-plastic among consumers may well be described by an ideal pattern. A model that assesses the extent to which sustainability-related decisions are made in an organization does not necessarily need to follow a pattern.

There are probably exceptions to a more general rule, but we see this aspect of the ODD as something in need of adjustment when tied to sustainability. Still, it is important to have a more concrete idea of where the model is aiming at and how to assess it. To maintain this and to make sure that the simulation remains valid across disciplines, we propose that scientists assess previously called patterns by using *propositions*. These are broad statements that resemble hypotheses but are stated in broader qualitative terms (see, for example, Cornelissen, 2017). There is no need to be too detailed in the *Overview* but one could present a few main propositions concerning the core area of the model (theory) – whether economic, social, environmental, or a combination of these – and then derive some (corollaries) to outline how the model connects to the other(s).

It is important that the propositions specify the connection between disciplines (when possible) and that they identify the nature of sustainability research. A step in this process is that of defining one or more outcome variables, i.e. those that constitute the target for the analysis of the simulated data. Even more important is that the measures, as defined in the propositions, are such that they can be used (and make sense) across disciplines. For example, monetary representations of the loss of variety in an ecosystem may not be appropriate to assess qualitative impacts. Vice versa, a biological account of variety may not be enough to fully understand the socio-economic effects of such a loss.

5.2. Entities and their characteristics

The second part of the *Overview* relates to entities, state variables, parameters, and scales (see Table 2). This part is still concerned with very general and static conceptualizations of a model, because it does not relate to the evolution of the system but with its basic components.

Table 2
Revised ODD specifications for sustainability.

Elements	Succinct explanation	Checks
1. Purpose	The general aim of the model.	(a) Are aspects of the triple bottom line considered? (b) How many disciplines are involved and which ones?
Propositions	A set of statements that indicate the direction in which the model is analyzed.	(c) How are outcome variables defined? (d) Are measures defined in one discipline easily interpreted from the perspective of others?
2. Entities	The basic components that define individuality in a simulation model.	(e) What is ‘agency’ for this sustainability research? (f) What should be excluded and why?
State variables	Numerical values that describe the entities.	(g) Are the choices dictated by data availability, knowledge of the phenomenon, or by opportunity?
Parameters	Coefficients and constants that operate on entities.	(h) What does it make sense to manipulate in light of the research question?
Scales	The extent to which the environment represents physical or abstract qualities of a space.	(i) Is the way in which the environment has been designed consistent with my sustainability stance? (j) Does the scale of time used capture the fast and slow timescales of sustainability?
3. Processes	The mechanisms in place to complete the operations in a computational simulation.	(k) Do processes operate within a disciplinary domain or do they cross domains?
Scheduling	The sequence with which processes are carried over.	(l) What would happen if the sequence is altered?

5.2.1. *Asking core questions: entities*

Reflections on the entities of an agent-based model are the most obvious and natural since agency is one of the core aspects of any such models. This is one of the advantages of using ABM in connection to sustainability because it forces modelers to actively identify the behavioral centers of the simulation. One of the main concerns in sustainability modeling is the fact that multiple actors dynamically interact and potentially play a role in affecting the outcome variable (Lang et al., 2012). A modeler should weigh the choice of whom/what to include and why. Moreover, by specifying agents' heterogeneity and autonomy, the researcher sets the conditions for the model to potentially identify emergent properties (Page, 2012, 2015). These factors are essential to the definition of complexity and seem essential in sustainability research too in that they allow for a better "structuration" of multi-level interconnectedness. There are two considerations here that reflect on the choice of entities and, at the same time, they also reflect on ABM in general.

The first consideration is about the possibility that an agent-based modeler has to describe the model with granularity of details and make it as complex as needed (Edmonds and Moss, 2005). This is a meaningful change from the mantra ‘keep things simple’ that is still valid for most modeling techniques. Of course, complexification comes at a cost and a modeler shall always ponder and choose carefully about what to include and how to do it. Sustainability modeling has the tendency to produce computationally heavy simulations, specifically because of the number and variety of agents involved and of the multi-layered interactions spanning on a variety of behaviors (e.g., economic, social, environmental). Hence, this feature of ABM is key to sustainability modeling. The good news is that complexity comes also with the benefit that the model is richer in structure and can thus be compared to a broad range of empirical observations, or patterns (DeAngelis and Mooij, 2005).

The second consideration is more abstract and pertains to the meaning of modeling from a philosophical point of view. When confronted with the choices of what to include in a model, every scientist is tasked with setting inclusion/exclusion criteria (Topping et al., 2015). This is unavoidable and constitutes part of what is called an act of "selective ignorance" (Magnani, 2017). In other words, by excluding parts of knowledge (e.g., a selection of stakeholders) the modeler is expressing an informed guess on what is more likely to affect the outcome variable (e.g., production of bio-fuel). How to set these criteria in sustainability ABM? This may vary from model to model, but those entities (e.g., stakeholders) that are more intertwined with the multi-layered nature of sustainability are probably those that should be included (see Table 2).

For example, in their model of decision making concerning land use in the face of environmental challenges, Le et al. (2012) define agents in a somewhat peculiar way. Their simulation environment is constituted of land agents and human agents. This is a very fruitful approach in that it clearly outlines the direction at which this sustainability research is aimed. At the same time, it begs questions of why the choice of these two agent types and not, for example, identifying agency in human beings (i.e. the decision makers), leaving the land more "passive" (environment-like). Or, to take an opposite stance, the land may be specified in a number of components (other agents) that, together and autonomously, interact with the human agent. Other questions may be asked on what was excluded by such a model. In modeling complex socio-ecologic systems, there usually are a number of variables and agents that are left out. In this case, for example, the configuration of the economy, social networks, decision history, and past policies may be considered. As stated above, the model does not *need* to include these agents. But a motivation as of why they were excluded may serve sustainability modelers well.

5.2.2. *State variables and parameters*

State variables can be also defined as the way in which entities are described. As such, this aspect cannot be separated by the one discussed in the previous sub-subsection. As per the ODD protocol, these are not to be confused with parameters. State variables are attributed to each entity and make it possible to distinguish one from the other. They can remain the same during the simulation's time or change according to it. Parameters are instead defined as "coefficients or constants used in model equations and algorithms" (Grimm et al., 2020b, S1: ODD Guidance and Checklists, p.8). Ideally, this is a good distinction[3] and it is useful in that it helps a modeler make sense of those aspects of the simulation that are manipulated in computational experiments and those that are not. Independent of how one structures a model, parameters are also very important when reflecting on a model, especially because they are key drivers to the analysis.[4] For this

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[3] Ironically, parameters can sometimes at the same time be state variables if the are used to distinguish agents. Growth rates for plants, or personality types for social models, can be parameters quantifying behaviors, but my differ, while being constant over time, among agents.

[4] How can we know which parameters we need without having detailed ideas about how to represent the model's processes? It might help here to say that in principle, each parameter is a sub-model by itself, it represents relationships. Growth rate, for example, as a constant parameter, is the most simple submodel we can think of, but we can also think of a very complex mechanistic model of how growth rate depends on all kinds of factors.

reason, and as a way to extend the roadmap we have decided to include the description of parameters in here. This is particularly relevant for at least two reasons. One is that setting a distinction between the two is also a way to help thinking about and structure a model. Ultimately the decision on whether an attribute (e.g., socially responsible behavior dispositions, attitudes towards working with sustainable suppliers) is a state variable or a parameters is a choice and this point in the roadmap may be the time to reflect on it (see Table 2).

Sometimes, there may be a choice between variables and parameters when forging the agents. After all, these are ways to describe the entities of a simulation and the modeler makes the choices here. These choices may be dictated by data availability, knowledge of the entities, or by opportunity. For example, in their model, Bravo et al. (2013) define their entities as consumers. Each one has a set of green products preferences P_i that are organized on four dimensions m. While preferences vary, the number of products (or dimensions) is fixed at 4. This is consistent with the literature and with keeping the simulation comparable with empirical data. However, nothing stops modelers from testing a number of cases where these dimensions take different values. The state variable and the parameter are intertwined in this case as they are in many other ABM. Hence, it makes it even more important to reflect on them.

5.2.3. Scales

Entities are also set to include the environment in which they interact. Whether it is a spatial representation of the target system or whether it is a mind-space (Secchi, 2022), it is worth considering when constructing a model. Many models in sustainability research are tied to actual geographical space (e.g., Yu et al., 2021; Madsen et al., 2021), but this is not a necessary condition. Being tied to geography or to an abstract space where proximity is an indication of cognitive, psychological, or social closeness is probably a signal about whether the model is tied more to environmental (the first case) or socio-economic aspects (the second case). For this reason, a reflection on the environment is already a statement on which of the three areas of sustainability constitutes a starting point for the model.

Within this element, *time* is another aspect that requires a few thoughts in the context of this paper. How is time conceptualized and what it means is probably a preliminary question that introduces what is to come under ‘processes’. As mentioned in the above sections, the dynamic of sustainable systems is particularly relevant because the assessment on any outcome variable needs to be based on time. By reflecting on whether a step in the simulation model has a correspondence to *actual time* (e.g., second, hour, year, decade) or whether it represents an *opportunity* (e.g., to interact, to make decisions, to assess the surroundings) has meaningful repercussions on how sustainability is conceived (for the latter, discrete-event scheduling, as often used in Operations Research, is a useful approach). Given the time pressures that humanity is currently facing it is understandable that modelers may prefer to focus on actual time. However, there are instances where opportunities – i.e. the availability of circumstances that potentially allow for action, thinking, behavior – are a better signal that the outcome variable can materialize. This is the case of a model on the factors that should align in order for households to understand which plastic is generic waste or recyclable waste. This is also particularly relevant in relation to the slow and fast timescales discussed above. In fact, a proper agent-based model of sustainable development should always take into consideration the two-way interaction between the here-and-now and the slower passing of time. Hence, this is a question to ask and definitely something to reflect upon when creating a model (see Table 2). Overall, the preceding discussion points to the necessity for ABM in sustainability to consider multilevel transmission mechanisms in the tradition of Coleman’s bathtub (or boat) model (Coleman, 1990). It conceptualizes linkages at the macro-meso-micro interface in a wide variety of social science computational models (Seri et al., 2022). A case in point here are sustainable behaviors. Reconsidering the previous example of household waste, macro-level national regulations for recycling will have an impact on how municipalities organize their waste management and also on individual behavior concerning household waste. Hence, our main argument is that modelers in the domain of sustainability ABM should bear those macro-meso-micro linkages in mind when setting their agents by explicitly thinking through what mix of aggregation levels is required. Especially in the sustainability domain, limiting the model to a single level appears to be insufficient for insight generation.

5.3. Processes and scheduling

The description of the model’s behavior is conducted through a definition of its *processes* (see Table 2). While the entities describe the structure of the model, the processes describe how this structure is changing within a given time step of the model, or at certain points in time. Here, *scheduling* refers to the sequence in which these processes happen: who (which entity) is doing what and when? Listing these processes, just by their names and a short description of what they are doing, is straightforward, but flow charts can be used if the scheduling includes many case distinctions. The list of processes would also clearly indicate which processes refer to social, ecological, or environmental processes.

The challenge here is that summary verbal descriptions of what is supposed to happen in a certain process, without providing details about how the processes are going to be implemented, is not sufficient for the purpose of OsDD. As Muelder and Filatova (2018) showed, verbal summary descriptions leave too much room for interpretation, and these interpretations can lead to completely different results. Therefore, in contrast to the original ODD, where the O-part does not include “details”, here we suggest to specify, using pseudo-code, algorithms including specific verbal statements, and, if needed, equations describing functional relationships. This would be challenging for non-modelers but, as we wrote in the Introduction of this article, OsDD is meant to be used by teams that include at least one experienced modeler. Ideally, the most important sub-models would be actually implemented and their behavior demonstrated. In general it is recommended to test sub-models separately (Railsback and Grimm, 2019). Here, even with sub-models being implemented, no claim would be possible on how, if taken together in a full model, the full model would behave.

By reflecting on the processes, one is asked to define the *mechanisms*. These are, according to many (e.g., Manzo, 2022), particularly important to understand causality. Not only agent-based models are structured around mechanisms (together with the environment and the agents Secchi, 2022) but these are pivotal mechanisms when they allow for emergent properties to appear. As already mentioned in Section 4.1, the way in which agents coordinate and interact in the *meso* domain is the key to understand how macro behaviors and patterns are linked to micro elements (if they are). As such, the configuration and combination of agents, along the interactions they engage in give rise to the apparent emergent complexity we see at the aggregate (macro) level. This is particularly relevant for any theory of sustainability, since there are multiple – and probably non-linear – combinations of social, economic, and environmental elements that contribute to sustainable development, behavior, thinking.

With research stemming across disciplines, the most difficult aspect of sustainability modeling (and theorizing) is to understand whether simulation processes span across disciplines or whether they are consistent within one discipline. Both cases may work fine, assuming the scheduling then explains why the sequence is designed the way it is and what would happen if it would change.

The first aspect mentioned about processes refers to the way in which they are usually designed. A process in a simulation is likely to be developed following an existing theory or conceptual model. Such theories and models are, unfortunately, very much embedded in single-disciplines. In Anebagilu et al. (2021), for example, the authors use the *theory of planned behavior* to study vegetative filter strips in the Larqui river basin, Chile. The processes related to the theory they used are consistent within the domain of applied psychology – the discipline from where the theory comes from. It is the scheduling of the simulation (the second aspect above) that connects the psychological process to the policies and the environmental conditions.

6. Concluding remarks

This article intended to demonstrate the potential use of ABM in developing sustainability theory. The starting point was that of acknowledging the wide diversity of conceptualizations around sustainability and assessing its status of an umbrella concept. Within this general framework, sustainability hosts a number of theories that are usually bound to one particular discipline and then transfigured into others. This has caused a lack of proper sustainability theory – since theory is always an adaptation from a specific discipline – and much vacuity in understanding what theory means in this domain of research.

We posit that theoretical advancements should come from embracing the characteristics (and needs) of sustainability research. On the one hand, time is a critical element, especially the way in which slow and fast timescales are intertwined. On the other hand, disciplinary diversity ought to be maintained since it is a key element to approach the complexity of the problems typical of this field. By maintaining disciplinary diversity, data issues may arise in terms of compatibility, source, and reliability. Another implication of the above is that sustainability research and theory need to make projections of current states to future states. In other words, it requires scenarios and analyses that are grounded in current data to extrapolate future trajectories in envisaging what constitutes a sustainable future.

The article advances the proposition that ABM could help sustainability address these critical elements and build theory in a more effective way. By asking questions related to the making of a model, the ODD protocol – especially the first part for which we propose the OsDD variant – help scientists reflect on assumptions, check their meaning, and develop a more robust (perhaps more consistent) determination of the aspects formalized in the simulation. Not only the questions allow reflections on the role of time, the use of multiple disciplines and the use of data but, in so doing, they also help with focusing specifically on the characteristics of sustainability.

The relation between models and theories has been explored many times in the past by philosophers of science (e.g., Magnani, 2017). Even though there is no final word on it, it is fair to state that models can be considered instantiations of theories. A modeling instrument and approach (ABM) that seems particularly apt to cover areas of a specific field of research (sustainability) has higher chances of making the transition to relevant theory more likely.

CRediT authorship contribution statement

D. Secchi: Conceptualization, Structure. **V. Grimm:** Ecology-related parts. **D.B. Herath:** Sustainability cases, ABM examples. **F. Homberg:** Sustainability cases, ABM applications.

Declaration of competing interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: One of the co-authors, Volker Grimm, is also one of the Guest Editors for the Special Issue ‘Agents for Theory’, Environmental Modeling & Software to which the article is submitted.

Data availability

No data was used for the research described in the article.

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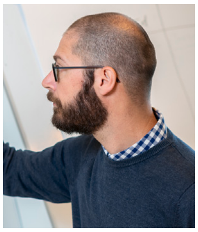

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