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Theory for and from agent-based modelling: Insights from a virtual special issue and a vision

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ABSTRACT

The Virtual Special Issue "Agents for Theory" discusses theory development using agent-based models (ABMs). The six contributions focus on how the word "theory" is used in the ABM literature, how reviews of ABMs should be conducted to gain general insights, how even the conceptualisation of ABMs can help to transform heuristic theories into scientific ones, how the context-dependent choice of decision models can be better justified, how reusable building blocks (RBBs) of ABMs could support theory development, and how a modular framework of RBBs can be used to identify general solutions. Overall, theories of decision making that go into ABMs and theories of system dynamics that come out of ABMs are interrelated, so the micro-macro perspective and the attempt to identify and reproduce patterns at both levels simultaneously is a way forward. Theory development requires clearer communication using a common language, reference to patterns, and more detailed model analysis and testing.

1. Introduction

Virtually all current major environmental and societal challenges such as climate change, loss of biodiversity, financial crises, migration, or erosion of democratic institutions, involve complex systems comprised of decision-making, adaptive agents. In such systems, individual actions and institutional policies may have unintended consequences that are hard to oversee or even predict (Schlüter et al., 2023). Analysing and understanding the dynamics of these agent-based complex systems (ACS) is one of the most urgent issues these days and essential for predicting their behaviour and management (An et al., 2021; Sargut and Gunther, 2011).

To understand how ACS function and respond to change and disturbances, agent-based modelling is increasingly recognized as the main way forward (Macal, 2016). Agent-based models (ABM) allow for a holistic view by linking different levels of organization (Gräbner, 2016; Iwanaga et al., 2021). By performing simulation experiments, one may find explanations for dynamics and developments, which would be too complex to oversee with other approaches. Strategies for developing realistic ABMs while limiting their complexity exist (Grimm and Railsback, 2012; Grimm et al., 2005) and are increasingly being used (Gallagher et al., 2021; Schmidt et al., 2023). Consequently, ABMs are of increasing relevance and we find applications in virtually all research fields including adaptive agents (Achter et al., 2024; Vincenot, 2018).

Still, notwithstanding the relevance of understanding ACS and the value of ABMs for accomplishing this goal, the method seems stuck in a stage of *ad hoc* model development and exploration. Besides all the merits of ABMs, scientific progress in agent-based modelling has been slower than expected. The majority of existing ABMs focus on specific systems, which limits generality. When designed to be more general, on the other hand, ABMs are often too simple and abstract to deliver testable predictions for real systems (Antosz et al., 2023). As a consequence, there is a 'call for theoretical engagement' (Lorscheid et al., 2019; O'Sullivan et al., 2016) pushing agent-based modelling into agent-based theory or even agent-based socio-ecology.

Since we simply cannot develop a new model for each and any ACS or upcoming detailed question, we need to identify and understand general principles, for example about the behaviour of their agents, their self-organization, their ability to cope with change and stress (resilience), and their propensity to catastrophic, sudden changes (regime

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shifts). Here, we refer to this search for general principles beyond single cases and contexts as 'theory development' to cope with the challenges of modern complex and highly interconnected ACS.

To discuss ways forward regarding theory development with ABM, we organized a series of three workshops, entitled 'From cases to general principles - theory development through agent-based modelling', funded by the Volkswagen Foundation and held in Hannover, Germany, in 2018, 2019 and, delayed due to the Covid-19 pandemic, 2021. While our background is in ecology and business economics, we were keen to discuss with leading ABM experts from a much broader spectrum of disciplines, including social sciences, economics, epidemiology, geography, anthropology, archaeology, philosophers of science, and epistemologists.

To summarize the main points and insights from our discussions, we invited, after the final workshop, contributions to this special issue in Environmental Modelling & Software. As a result, we have six contributions (Table 1) that address important aspects of theory and its development, provide insightful reviews, and discuss possible ways forward. In this editorial, we are summarizing their main points.

With this editorial, we aim at an in-depth summary of the six contributions to the special issue, in the style of a 'readers digest'. Thereby we are trying to provide a roadmap for further reading, as each of these contributions is full of important findings, ideas, and suggestions. Also, in the end, an attempt is made to provide a general conclusion and a discussion of the most promising ways forward toward theory development with ABMs.

Table 1
Content, topics and insights addressed by the six papers included in the Virtual Special Issue "*Agents for Theory*".

Title	Topics and insights	Authors
What do you want theory for? – A pragmatic analysis of the roles of 'theory' in agent-based modelling	- How is the word 'theory' used in the ABM literature? - Most often, 'theory' is used for agent decision models. - Testing such theories in ABM requires additional assumptions, which limits their generality.	Antosz et al. (2023)
How to conduct more systematic reviews of agent-based models and foster theory development – Taking stock and looking ahead	- A review of reviews of ABMs. - Recommendations for systematic literature reviews. - Defines seven theory dimensions. - Shows that important theory dimensions are rarely addressed in ABM reviews.	Achter et al. (2024)
Modeling and theorizing with agent-based sustainable development	- Verbally formulated theories leave too much room for interpretation. - Agent-based modelling allows us to translate heuristics into scientific theories. - Even just being explicit about the entities, variables, scales, and processes involved would provide a common language and reduce ambiguity. - A modified version of the O-part of the ODD protocol could be used for this.	Secchi et al. (2024)
Agent decision-making: the elephant in the room - enabling the justification of decision model fit in social-ecological models	- Most decision models in ABM still assume the *homo oeconomicus*. - The choice of the decision model to be used depends on the context defined by the ABM. - Five existing frameworks that help make this choice are compared. - A survey of the practice of modelling decision-making is presented.	Wijermans et al. (2023)
Towards reusable building blocks for agent-based modelling and theory development	- Introduces the concept of atomic Reusable Building Blocks (RBBs) as effective tools for ABM theory development. - Provides a workflow and tools for sharing RBBs. - Illustrates the RBB concept to foster discussion and encourage refinement.	Berger et al. (2024)
A platform for plant-growth modellers: python models for agent-based resource gathering (pyMANGA)	- A modular software platform is presented, as an example, that includes alternative building blocks representing resource use and allocation, growth, and competition of trees, or plants in general	Wimmler et al. (2024)

2. ABM fosters the formalisation of theories

Complaints about limited theory development with ABMs are justified, but it should not be forgotten that without ABMs most of the plethora of verbally formulated theories dealing with human behaviour and social phenomena will remain vague and untestable. The quest for more theory development tends to come from disciplines with some established computational or modelling background, such as ecology, economics, or geography, and a long tradition in mathematical formalizable modelling approaches. The social sciences, on the other hand, seem to have too many 'theories' (Secchi et al., 2024), which usually are verbally formulated assumptions about certain mechanisms. Calling them theories, and giving them a name, helps to turn them into 'memes' that are easier to remember and therefore easier for others to refer to, thereby increasing the impact of their developers.

However, verbally formulated theories are too ambiguous to be tested and further developed (Muelder and Filatova, 2018). Secchi et al. (2024) claim that this has been limiting theory development for ACS because 'the definition of mechanisms, assumptions, dynamics and the determination of the entities involved are largely left to the reader's imagination' (p. 1). The authors distinguish between 'heuristic' theory, which is an assumption or hypothesis of how certain observations could be explained, and 'scientific' theory, which is an explanation of observations that is supported by vast evidence.

They specifically describe the situation in sustainability science, where numerous heuristic theories exist, both about theories of behaviour and about the mechanisms behind the dynamics, robustness, resilience, or vulnerability of a coupled human-environment system. They include expressions that may have different conceptualizations, or, vice versa, concepts that are referred to with different expressions. This ambiguity is particularly prominent in sustainability science because it involves different disciplines, all with their concepts and terminology. Secchi et al. (2024) argue that implementing these theories in ABMs would make them more specific and explicit. ABM can explore how system-level elements such as norms, values, and cultures are mutually linked to the behaviour of agents. They can represent processes on both slow and fast time scales, and how they affect each other. They can capture nonlinear effects and provide output that can be rigorously analysed using quantitative methods and statistical inferences.

However, since developing and analysing ABMs requires time, effort, and modelling expertise, translating all verbal theories, in all possible contexts, to ABMs remains impossible. The rationale of ABMs can still be used powerfully because heuristic theories can be translated into the design of an ABM, even if it is not implemented and run. For this, Secchi et al. (2024) recommend a slightly modified version of the so-called Overview part of the ODD protocol which became a standard for the description of ABM (Grimm et al., 2006, 2010, Grimm et al., 2020; Polhill, 2010; Polhill et al., 2008).

ODD comprises seven elements. The first three, grouped in the Overview part, 'Purpose and Patterns', 'Entities, State Variables, and Scales', and 'Process Overview and Scheduling', are meant to provide a quick overview of the ABM's purpose, structure, processes and scales. This overview allows readers to embrace the entire ABM before turning to details of how the model is initialized, what data are imported, and how the processes are implemented in detail. These details are provided in the ODD elements 'Initialization', 'Input Data', and 'Submodels'. The ODD elements listed so far, which describe the model, are augmented by the element 'Design Concepts' that comprises 10 concepts that are important to explicitly consider when designing an ABM, for example, 'emergence', 'interaction', or 'observation'.

We agree with Secchi et al. (2024) that formulating ODD-style overviews of heuristic theories for ACS would force us to be explicit about the entities, variables, processes, and scales that we believe to be relevant and sufficient for explaining certain phenomena. Of course, the insights to be gained from such overviews are limited, as only the fully implemented model would allow us to test rigorously if, how, and under which conditions our theory holds, but still, the overview would provide a means for communication across disciplines by providing a unifying structure and terminology. The unifying potential of ODD has already been demonstrated in a bibliometric analysis (Vincenot, 2018) but could be even more powerful in the proposed manner.

Secchi et al. (2024) slightly modify the original ODD overview to accommodate it to the specific challenges of sustainability science (Secchi et al. [2024], Table 2). Overall, Secchi et al. (2024) remind us that with complaints about limited theory development with ABM, we should not *throw out the baby with the bathwater*. ABM is an indispensable approach when it comes to dealing with ACS. We need ABM, but we also need to make their design, analysis, and use more efficient and coherent, and to more directly and explicitly aim at the development of more general concepts and principles (Grimm and Berger, 2016a; Lorscheid et al., 2019). Using a unifying terminology and structure not only for communicating but also for designing models would make ABM more efficient and coherent. The ODDs overview suggested by Secchi et al. (2024) provides such unifying terminology and structure and thereby fosters integration and theory development in sustainability science.

3. How is the term 'theory' used in the ABM literature?

Our workshops started with the premise that theory development with ABM is too limited to sufficiently understand and manage ACS. However, this does not mean that we were the first to address theory development with ABM, or that the word 'theory' is not used in the ABM literature, as pointed out by Antosz et al. (2023). The potential of ABM to develop theory was described decades ago, e.g. for ecology (Huston et al., 1988) and organization theory (Anderson, 1999; Carley, 1995) or, more recently, analytical sociology (Hedström and Ylikoski, 2010). The term 'theory' has since been used in the literature, and Antosz et al. (2023) wonder how and why it is used, but first they provide a list of different connotations of 'theory'.

On the one hand, according to Antosz et al. (2023), a *scientific* theory should have some degree of generality, contain some causal explanation, be intelligible to humans, usually be a relatively high-level description, and be empirically testable. It can be used to make inferences about phenomena, posits a new entity, and is formally expressed, for example, using mathematics. Of course, not all scientific theories have all of these characteristics, but they do have some of them. On the other hand, a theory may only be *heuristic*, i.e., according to Antosz et al. (2023), it may be vague, may not constrain possible explanations very much, may assume a certain context, may require further assumptions to make it testable, and maybe a way of thinking rather than a causal or mechanistic explanation. Thus, people mean different things by 'theory' and refer to it for different reasons.

Antosz et al. (2023) searched articles from three leading modelling journals in social, environmental, and spatial sciences, respectively, which had the word 'theory' in the title, abstract, or keywords. Most of the articles they found, e.g., in environmental modelling, use the word 'theory' because the ABMs in these articles include one or more theories from other domains to represent the *decision-making* of the agents, such as evolutionary game theory or the *Consumat framework* (Jager and Janssen, 2012). By using existing theories, model developers reduce the burden of justifying the design of the entire ABM as they use those theories as building blocks that seem to have some status of being established, realistic enough, and of proven explanatory power. This practice has been criticized before by (Sun et al., 2016), who found that theories are often used in models to camouflage the lack of knowledge and data (referred to after Taghikhah et al. (2021)).

In principle, using existing theories of decision-making in an ABM could lead to theory development, by systematically exploring how alternative versions of a theory of decision-making affect the predictive power of the entire ABM, i.e. the ability to reproduce one or more observed patterns ('pattern-oriented theory development'; An et al., 2021; Grimm and Railsback, 2012; Railsback and Harvey, 2020). This is rarely done, however, and even if it has been tried to some degree, Antosz et al. (2023) are afraid that the resulting theory development will be limited, because 'the theory incorporated is only tested along with a host of other assumptions' (p. 4).

This is a key challenge of theory development with ABMs: context dependency. Unlike in physics, where universal theories, dubbed 'laws', exist, the set of constraints affecting the behaviour and decisions of agents varies widely in space and time, but how the theories of these behaviours deal with these constraints is usually not fully specified. Most ABMs that claim to represent real systems have to focus on a specific context in space and time, otherwise they cannot be verified and validated. Theory development, however, requires applying theories for a whole range of contexts, which is of course limited by time, data, and resources. One possible way to reduce context dependency is to aim for theories of behaviour that are so basic, or 'atomic', that they are likely to hold for a wide range of contexts (Berger et al., 2024). The systematic search for 'reusable building blocks' (RBBs; Berger et al. (2024)) can help in compiling such basic theories, but the context will always play a role. In our view, there is a need for context to be more systematically considered in theory development with ABM. A first condition for this is to clearly communicate this context and how it might affect the application domain of a theory. Antosz et al. (2023) summarize their review of the use of the word 'theory' in the ABM literature by making the distinction between a theory that goes 'in' to an ABM, and a theory that comes 'out' of an ABM, i.e. 'what is assumed compared to what is inferred' (p. 7). Getting more theory out requires first of all always carefully distinguishing between 'heuristic' and 'scientific' theory.

As a way forward, Antosz et al. recommend either starting from a set of empirical, i.e. data-driven, models for a certain class of system and then trying to identify commonalities, possibly via machine learning. Alternatively, an empirical model could be replaced by a statistical meta-model (e.g., Lafuerza et al. (2016)), which then could be simplified to see at what point it loses its explanatory power. This approach to reducing context-dependency is similar to the Robustness Analysis suggested by (Grimm and Berger, 2016b), which does not employ meta-modelling but is based on a systematic simplification of a model 'to separate the scientifically important parts and predictions of our models from the illusory ones which are accidents of representations' (Weisberg, 2012).

4. How more systematic reviews can foster theory development

Achter et al. (2024) believe that 'literature reviews of ABMs may foster learning beyond individual cases and encourage theory development by stimulating the discovery of general patterns at the system level and aligning modelling conventions at the agent level' (p. 1). Achter et al. (2024) focus on the potential of Systematic Literature Reviews (SLR), which is an established approach but has not yet been used for the review of ABMs. Achter et al. (2024) suggest a minimum standard for SLRs of ABMs. The additional workload for complying with these standard practices needs to be considered when planning a review, but the added value both for those carrying out the SLR and for theory development, in general, can provide sufficient payoff. Example reviews fully complying with their standard are DeAngelis and Diaz (2019), Magliocca (2020), Matthews et al. (2007), Lorig et al. (2021), and McAlpine et al. (2021).

Achter et al. (2024) then suggest seven dimensions along which ABM reviews can contribute to theory development (Achter et al. [2024], Table 2.3). The first two dimensions are used to compare the structure and the processes of ABMs. This would be facilitated if all ABMs were described in the same way, for example using the ODD protocol (McAlpine et al., 2021), whose elements two and three ('Entities, State variables and Scale', 'Process Overview and Scheduling'), correspond to these two dimensions. Dimensions three and four are about the verbal and formal description, respectively, of the theories implemented in an ABM. The remaining three dimensions are trying to go beyond single cases and ABMs. They focus on generalization by identifying common elements of theories addressing the same phenomenon, and by identifying blind spots of important, but rarely addressed issues; generalization can also be the explicit goal of a review, in the sense of 'What have we learned?'.

Achter et al. (2024) use these seven dimensions in their own SLR of ABM reviews. They found 127 ABM reviews across all disciplines but then focussed on 29 reviews from ecology and 13 from the social sciences. They scanned these 42 reviews for the seven dimensions by which reviews could contribute to theory development (Fig. 1). Obviously, the coverage of dimensions is diverse and generally incomplete. In particular, they found a stronger focus on reviewing the design of ABMs than on the insights that were gained with them. They describe in detail the most valuable reviews, both to summarize their findings and to demonstrate that it is possible to use reviews to support theory development.

They conclude their review of reviews with the belief that it 'provides authors, reviewers, and editors an anchor point for advice and discussion' (p. 17). They also highlight the potential of using standards, like the ODD and ODD + D protocol, and of using bibliometric methods, to make reviews more useful. Their main conclusion, however, is that the missing 'focus on the insight perspective indicates the enormous potential of future ABM reviews' (p. 19).

5. Theory in: which decision-making model to use, and why?

As documented in the review by Antosz et al. (2023), theories of decision-making are widely used in ABMs, as decision-making determines the behaviour of humans and their institutions, but also of organisms (Railsback and Harvey, 2020). Although there is a wide range of such theories, most ABMs represent human decision-makers 'as simplified, perfectly informed, rational optimisers, without explicitly considering the decision context' (Wijermans et al., 2023). This bias towards this *homo oeconomicus* of neoclassical economics led Wijermans et al. (2023) to wonder how modellers decide which decision model to use. Interestingly, it appears that the terms 'theory' and 'model' seem to be used interchangeably in the context of agent behaviour, whereas the difference between these two terms is hotly debated for ABM as a whole (Antosz et al., 2023).

Wijermans et al. (2023) start from the premise that we need to better understand which decision model (DM) is most appropriate in a given context, to better align with the overall purpose and questions of the ABM. There are indeed contexts and purposes where the *homo oeconomicus* would be an appropriate DM, but how can we define and categorize contexts and purposes? The authors suggest that modellers of social-ecological systems (SES) learn to navigate in the landscape of different DMs and that they consider alternative options, for example by considering theories from the social sciences, which, as we have learned from Secchi et al. (2024), are abundant. To facilitate all this, Wijermans et al. (2023) describe existing frameworks for orientation in the DM landscape, and provide guiding questions that help to find the best DMs for a given context.

The frameworks characterized by both their strengths and weaknesses are: 1. Agent decision architecture dimensions (Balke and Gilbert, 2014), where six dimensions are defined to compare different DM architectures; 2. Varieties of Rational Choice Microfoundations (Wittek et al., 2013), where the three DM dimensions rationality, preferences, and individualism are distinguished; 3. Model Social Agent (Carley and Newell, 1994), where the agent's knowledge and the limitations of the

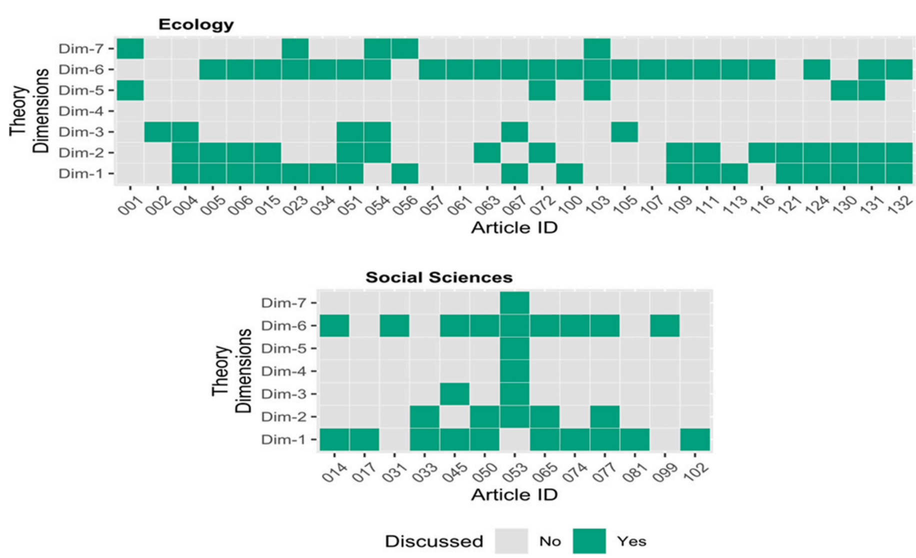

Fig. 1. Results of a review of ABM reviews (Achter et al., 2024) from ecology and social sciences regarding the coverage of seven theory dimensions (see main text for details). While certainly not all reviews can or should cover all dimensions, it seems that some important dimensions tend to be ignored in general (from Achter et al. (2024)).

processing capabilities are emphasized; 4. The Contextual Action Framework for Computational Agents (CAFCA; (Elsenbroich and Verhagen, 2016), where nine decision modes are defined by a matrix of three types of reasoning used, i.e. habitual, strategic and normative, and three social dimensions, i.e., individual, social, and collective; 5. MoHuB and HuB-CC frameworks (Constantino et al., 2021; Schlüter et al., 2017), where concepts for describing and comparing DMs are provided, such as perception, behaviour, situational and stable characteristics etc.).

Wijermans et al. (2023) decided not to add their framework, as the existing list, which they do not claim to be exhaustive, can be confusing enough. Instead, they recommend that SES modellers familiarise themselves with the existing frameworks and try to see how they can help in deciding which DM to use in a given context. This includes not only choosing a particular DM architecture but also positioning the chosen DM in the landscape of alternatives by being clear about what a certain DM can and cannot do. In addition, these five frameworks, and in particular the different dimensions that define context, should be used to evaluate and challenge the DM choice of others, for example when reviewing an ABM. As considering all five frameworks can be challenging, Wijermans et al. (2023) provide a list of questions that help to be explicit about the context of the DM being developed or evaluated (Fig. 2). In addition to looking for the most suitable DM for a given ABM and context, Wijermans et al. (2023) recommend looking for existing DMs beyond the modeller's own comfort zone.

We are not sure if indeed a 'plethora of different theories are ready for use', as most theories in the social sciences are presented verbally; but indeed one would ideally be able to select from a broad spectrum of DMs that are implemented as Reusable Building Blocks (RBBs; see the following section on the contribution by Berger et al. (2024)).

To support getting an overview of DMs that are being used in ABMs, Wijermans et al. surveyed social simulation modellers, with 117 responses. The results show that in contrast to current practice across all disciplines, most social and SES modellers go beyond the *homo oeconomicus*. For example, more than 70% of the respondents considered including memory, goals, influence of others, and learning as being part of their current practices. Wijermans et al. discuss in detail the state of the art, and the challenges, related to who's decisions are modelled (individual agent, group of agents, or institutions), how the DM's context can be characterized, how learning is represented, and if and how machine learning can provide useful DMs. For each of these topics, they discuss specific examples from the literature.

Probably the most important of these challenges is the context of DMs. Context is defined by Wijermans et al. as 'a container term consisting of all things around the agent that it is made aware of and/or sensitive to (Edmonds, 2012))'. Its main dimensions are the specific time and region addressed by the ABM, the problem being modelled, and the environment, i.e. all external factors, including both biophysical and social ones (often referred to as the scenario). Making this context explicit, ideally in a standardised way, would allow us to compare the design and findings of ABMs more systematically. The use of standard formats for describing ABMs, such as ODD or, in this context, ODD + D (Müller et al., 2013), should be sufficient to describe the context in detail, but how the context determined which DM was used is not yet explicitly addressed in these standards. It should also be noted that there are already DMs that include options for a wide range of contexts, such as *Consumat* (Jager and Janssen, 2012; Jager et al., 2000).

Wijermans et al. (2023) see the purpose of their article as raising awareness of the different dimensions that influence the choice of DMs and the range of DMs that, in principle, exist. They make it very clear that all this is not intended to make agent-based modellers defend the DM they use as the best one but as a suitable one for a given context. All this has great potential to improve the state of the art of agent-based modelling, especially in social and socio-ecological simulations, and to facilitate the development of theories of human decision-making.

6. Reusable building blocks – RBBs – for ABMs

A major obstacle to theory development with and for agent-based modelling is the fact that most ABMs are still largely developed from scratch. This makes it difficult, if not in many cases impossible, to learn from systematically comparing different ABMs, even if they include the same processes or behaviours and address similar systems and questions. Berger et al. (2024) therefore seek to promote the development and routine use of reusable building blocks (RBBs) for ABMs.

RBBs are not a new idea. They are used in software development, for example for developing computer games. Also, the huge success of the statistics software platform R (Core Dev) is due to its modular design. Transferring this idea to modelling, however, turned out to be challenging. Berger et al. (2024) refer to the literature, especially from the

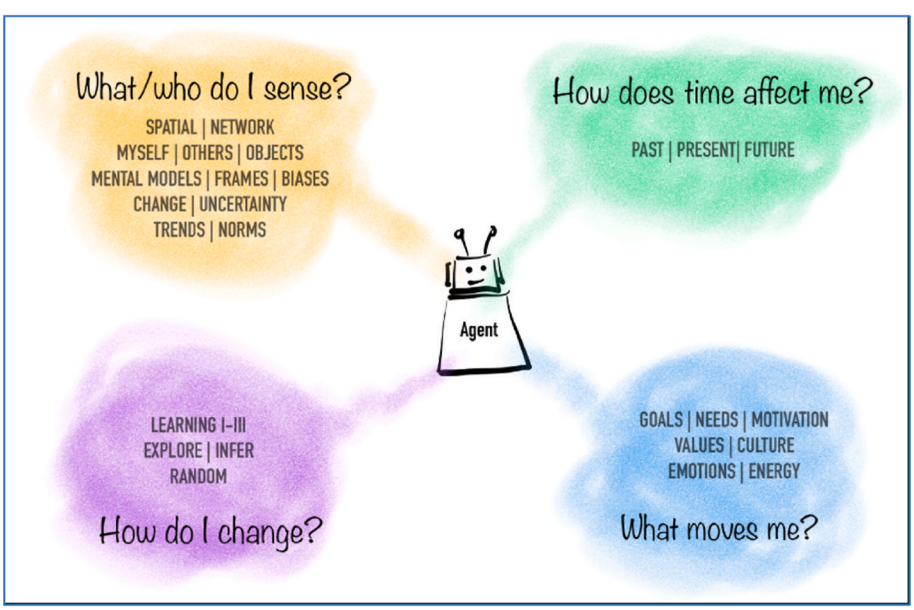

Fig. 2. Guiding questions that help agent-based modellers to clearly define the context of the decision model that they want to use in their ABM (from Wijermans et al. (2023)).

domain of 'Modelling & Simulation', which is mostly about complex models for large applications in business and industry. There, all attempts to establish modular systems of building blocks seem to have failed, with one exception, a platform for simulating battles (High Level Architecture; Dahmann et al. (1997)).

Berger et al. (2024) see a main problem in the vague meaning of 'module', which can range from whole complex submodels, such as the foraging model in the honey bee model BEEHAVE (Becher et al., 2014), over more or less complex models of certain mechanisms, to extremely simple models of very specific behaviours. The more complex a module, the more likely will its functioning depend on the context of the entire ABM. For example, how farmers buy and sell land will depend on how the market for land is organized, on national or even regional regulations, on cultural norms, etc. Thus, a module working fine in a certain region, at a certain time, and for addressing a certain question, may lead to wrong results in a different context. This is well known for entire models, where coupling them can lead to 'integronsters', i.e. new models with unrealistic behaviours, which are also hard to understand (Voinov and Shugart, 2013).

According to Berger et al. (2024), the only solution to make RBBs a living and useful concept is to minimize context-dependency as much as possible by focussing on 'atomic' building blocks. They define an RBB for an ABM to be 'a submodel that represents a particular mechanism or process that is relevant across many ABMs in a certain application domain.' (p. 2). This definition narrows the scope of an RBB to a certain application domain, for example, plant competition or planned behaviour. Even within this confined context, Berger et al. emphasize that the vision of plug-and-play of RBBs is unrealistic. Rather, it has to be checked in detail for which context an RBB was developed and if using it in a different one would require amendments.

While this openness to change seems to contradict the very idea of a reusable building block, it actually can contribute to developing theories of certain behaviours, in particular, decision models; Wijermans et al. (2023) explicitly suggest using decision models in different contexts and systematically compare them and the resulting ABM outputs. This process of theory development across different contexts can sometimes lead to a real 'atomic', context-free RBB, but in other cases to a pedigree of RBBs of the same process in different contexts. For example, the original zone-of-influence approach for describing plant competition is still used for many questions but has also been developed into a more realistic approach (Field of neighbourhood, Berger and Hildenbrandt, 2000), or extended to take into account above and belowground competition separately from each other (Lin et al., 2014; May et al., 2009).

Moreover, testing alternative versions of an RBB for their potential to reproduce a whole set of observed patterns ('Pattern-oriented modelling'; Grimm and Railsback (2012); Grimm et al. (2005)) can not only help find the most suitable version for a given context but has the potential to identify general behavioural principles. In ecology, this has worked already in several cases, for example for models of animal energy budgets (Kooijman, 2010; Sibly et al., 2013), habitat selection (Railsback and Harvey, 2002; Railsback and Harvey, 2020), or foraging of vultures (Cortés-Avizanda et al., 2014).

However, to achieve a critical mass of RBBs so that modellers routinely refer to them, several challenges need to be addressed: 1) development, 2) sharing, 3) verification, and 4) reuse of RBBs. Development requires that the RBB is presented in a way that it can be used independently of the specific programming language with which it was developed. This, in turn, requires a non-technical description, e.g. using ODD, but also a narrative description of its purpose, application domain, behaviour, and limitations. Sharing and reviewing RBBs requires curated web repositories, and using an RBB requires careful configuration (Lorscheid and Meyer, 2016) and documentation for the intended context.

The main motivation for contributing RBB to some peer-reviewed repository is that the RBB can get a *doi* and is thereby made permanently accessible and citeable. To prepare such a repository, Berger et al. present a first template that includes the RBB and the corresponding information in a standardized way. To keep the bar low for submitting RBBs to a repository, their template includes a minimum standard, but also a full one, which requires more effort to meet but also makes the RBB easier to understand and use. For demonstration purposes, Berger et al. developed a temporary webpage, www.rbb4abm.com, but a fully developed and more comprehensive one will be released in spring 2024 (see link then on www.rbb4abm.com).

Despite all the undeniable benefits of having a system of RBBs available, it remains challenging to reach the critical mass of RBBs. Most promising are community efforts, where certain interest groups agree on which RBBs would be important to have, and then jointly develop them, and ideally make them available via the planned RBB repository, which then could have certain disciplines or application domains as tags of the RBBs. Examples of such community, or working group, efforts are Community Surface Dynamics Modeling System (CSDMS, https://csdms.colorado.edu/wiki/About_CSDMS) or pyMANGA (https://github.com/pymanga; Wimmler et al. (2024)) which provides various RBBs including ZOI and FON to assemble plant population models. Ultimately, however, the success of RBBs, and hence their contribution to theory development, depends on the motivation of individual modellers to invest the effort for sharing their own, or an existing, submodel as an RBB, and to make sure they get a sufficient return in terms of citation and recognition for this contribution.

7. pyMANGA: an example of a modular system for modelling and theory development for forest and vegetation dynamics

In forest ecology, individual-based models (as ABMs are usually called in ecology) have a long tradition, going back to the pioneering so-called gap model JABOWA (Botkin et al., 1972), which has led to a whole pedigree of forest ABMs with all kinds of modifications and extensions (Fischer et al., 2016; Shugart et al., 2018). All these models, as noted by Wimmler et al. (2024), have to deal with 'the same processes, namely tree establishment, growth and mortality, and competition for above- or below-ground resources' (p. 1), but there is a great deal of variation in how these processes are represented in detail. The choice of representation should ideally be determined by the question being addressed and the data and knowledge available, but in practice, the preferences and experience of the modellers involved also play a role, as do modelling traditions in particular fields of application.

Theory development about these processes at the level of individual trees and the forest scale would be greatly facilitated if there were a modular system in which different representations could be easily combined and contrasted. This would allow us to test what we gain or lose from more complex representations, where the limitations of particular representations lie, and what combination would be most appropriate for a given model purpose and context. Wimmler et al. (2024) have developed a modular system, called pyMANGA (https://github.com/pymanga), which originally emerged from their work modelling mangrove forests. Within pyMANGA, reusability, as defined by Berger et al. (2024), of all building blocks is a defining feature. Even plug and play of alternative building blocks, e.g. of the growth or competition model used, is possible because the overall context, forest and vegetation growth, is relatively narrow, and well-defined.

The authors see pyMANGA as 'a community-based platform that provides the infrastructure to allow model ideas, especially from small projects, to persist and be reused in future projects' (p. 2). They made sure that the interfaces between the different modules or building blocks were designed to be generic. For example, for mangroves, it is only important to obtain values for pore water salinity, not whether these values are provided by a detailed mechanistic soil water model or a phenomenological model. Transparency and traceability are achieved by implementing pyMANGA in the version control system 'git', a software that also facilitates collaboration and will therefore play an increasing role in agent-based modelling. As far as automation is concerned, not only source code documentation is automated, but also unit tests and benchmarks.

In a demonstration, the authors use pyMANGA to model the dynamics of a small plot of black mangroves (*Avicennia germinans*) for which data on tree density, stem diameter, and age are available. They examine how all four possible combinations of two sub-models describing below-ground resources and their uptake, and two sub-models describing tree mortality, fit together. Each of these sub-model pairs has a simple and a more complex version. The authors found that it was sufficient to include either the more complex resource model or the more complex mortality model to obtain realistic results. This supports once more the interesting question of whether, for the description of real systems, we should always search for only one dominant mechanism to underlie observed phenomena, or whether we should assume multiple, interacting causes. In the pyMANGA example, the data, or observed patterns, are not sufficient to decide which of the two complex submodels was dominant in reality, of if even both had to interact.

pyMANGA is an open platform, and the authors invite peers to participate not only to use it but also to contribute their models of resource distribution and allocation and plant competition. While the benefits of doing so are clear, some investment is required, as the platform requires the use of the Python programming language and the git version control system, as well as the writing of the scripts needed to implement all the necessary workflows.

But when it comes to collaborative work and theory development, there is no such thing as a free lunch. Most modellers in ecology, and probably in the social sciences, are more or less self-taught programmers who know just enough about programming to make their models run and be used, but this limits the use of existing computer science and software engineering tools. On the other hand, even if only two or three different working groups agreed to use a platform like pyMANGA, both individually and collaboratively, the critical mass of both users and reusable building blocks available within this platform could quickly be reached. Thus, the development of modular platforms such as pyMANGA, designed for well-defined classes of systems and questions, could be a solution to the major challenge of establishing the development and use of reusable building blocks (Berger et al., 2024).

8. Discussion and synthesis

8.1. The different dimensions of theory

The Virtual Special Issue 'Agents for Theory', and the series of workshops from which it emerged, started from the observation that ABMs of ecological, environmental, and social systems (here simply called ACS), and their combinations, tend to be case-specific. Despite the considerable effort that goes into their development, the insights gained from them are seldom transferable to other cases. This needs to change. We cannot afford to develop a myriad of ABMs, particularly not in the light that all these systems are currently changing so rapidly that case- and context-specific models may soon become obsolete. Furthermore, as scientists, we are naturally motivated to seek predictive understanding based on general principles. While this intrinsic motivation is certainly stronger in the natural sciences, it also exists in the social sciences, although often tempered to more modest goals, such as 'middle-range theories', a popular concept in sociology (Merton, 1968; Schlüter et al., 2019).

The underlying theme of this special issue is how to move 'from cases to general principles'. We have called this 'theory development', which in retrospect may not have been the best idea, since 'theory' itself is a fuzzy concept. As with other fuzzy concepts such as stability, resilience or sustainability, however, the only way to move forward is to define what we mean by these terms in a given context and to acknowledge that there are different meanings, often for good reasons.

As far as agent-based modelling is concerned, we seem to have to distinguish between two types of theories: 'scientific' and heuristic (Antosz et al., 2023; Secchi et al., 2024), and between two levels addressed with them: theories of decision making and behaviour, and theories of the dynamics of the ACS (Antosz et al., 2023; Wijermans et al., 2023). The main characteristics of 'scientific' theories are that they have some degree of generality, reveal causal relationships and have empirical support, whereas heuristic theories are assumptions, hypotheses, concepts or conjectures, typically expressed verbally, not formally and therefore not testable (Antosz et al., 2023; Secchi et al., 2024). Both types of theory are important and necessary in science, which is why we put 'scientific theories' in quotes, but when it comes to identifying general principles underlying the behaviour of agents or the dynamics of ACSs, heuristic theories are not sufficient and need to be translated into 'scientific' theories.

Agent-based modelling is a key approach for this translation (Secchi et al., 2024). The potential of ABMs to develop and even 'unify theory' (Huston et al., 1988) has been known for a long time (see references in Antosz et al. (2023)), but obviously, there are challenges.

8.2. Learning from each other

Reviews are an important tool for advancing science as they summarize the state of the art in terms of methods and findings, identify gaps, and suggest priorities for further development. For agent-based modelling, there are more than a hundred reviews, but most of them are not systematic enough and focus too much on the design of models and not enough on the insights gained from the models (Achter et al., 2024).

For future reviews to be more useful, the guidelines and examples provided by Achter et al. (2024) are most helpful, but this special issue shows that the various suggestions for improving theory development are all interrelated. Without better communication of context, assumptions and choices, we cannot move forward, but 'better' means standardisation, which means acceptance of best practice, which requires evaluation through systematic reviews, etc. (Hauke et al., 2020).

8.3. Testing 'theories in'

When explicitly referring to 'theory', in ecology this is mostly about the system level (Grimm, 1999), whereas in the social sciences, it is mostly about the level of agents' behaviour and decision-making (Antosz et al., 2023; Secchi et al., 2024). Most of the latter are verbally formulated and thus heuristic. Trying to formulate them formally, using common terminology and structure, would reduce their ambiguity (Secchi et al. (2024)).

While formally represented theories certainly would support theory development, they need to be implemented and tested within ABMs. Here, the next challenge is that often, e.g., theories of decision-making in an ABM are just taken as given building blocks, without testing their explanatory power and limits within the ABM. This may be so partly because there is just not a culture for doing so (Schulze et al., 2017), but also because one might assume that such testing would require too many additional assumptions to allow for generality (Antosz et al., 2023).

This issue of context dependency was highlighted as a major challenge also by Wijermans et al. (2023). There is no 'one-size-fits-all' theory of decision-making, and various existing frameworks can help find the best decision model for a given context, as summarized by Wijermans et al. (2023). This does not prevent the development of theories of decision-making. Rather, the context should be clearly communicated and the choice of the decision model used in an ABM should be justified (Wijermans et al., 2023).

8.4. The key role of communication

The lack of clear and comprehensive communication of the details and assumptions that matter is a common theme in virtually all the papers in our special issue. Models expressed in terms of equations or algorithms may appear rigorous or 'scientific', but their development is not. Simulation models such as ABMs are not derived mathematically or strictly logically, but are based on heuristics, tradition, trial and error, and not least on the personal preferences, skills and experience of their developers. While all of this is inherent to modelling, it does not mean that we should not be transparent about context and assumptions.

A way forward is using a common language, in addition to the language of equations and algorithms. ODD is the most widely used common language for ABMs so far, and for theories of human decision-making, ODD + D is increasingly used (Müller et al., 2013). ODD + D already includes many aspects that force us to describe in some detail the decision context and the reasons why a particular DM was used. Still, using a certain standard format does not guarantee that it has been used correctly and that it allows us to improve theory development. Like with ODD (Grimm et al., 2010; Grimm, 2020), a review of existing ODD + D uses might be needed, to check for compliance and possible misunderstandings. Moreover, an update taking into account the findings and recommendations by Wijermans et al. (2023) might be useful.

However, standards for communication may not be enough. The word 'standard' has three main connotations in the context of modelling: a common way of doing things (such as the QWERTY design of keyboards), a good practice (such as good laboratory practice), or a minimum standard for quality assurance (such as minimum standards for writing tests). Ultimately, moving from cases to general principles with ABMs will require standards that cover all three of these aspects. ODD and ODD + D are a start, and there are initial attempts to define good modelling practice. (Grimm et al., 2014; Hamilton et al., 2022; Planque et al., 2022; Schmolke et al., 2010), but it will need time and a major community effort to develop, establish, evaluate, and update such standards. The Open Modeling Foundation[1] (OMF) recently started working on all this (Barton et al., 2022) and certainly has the critical mass for supporting the standards to be developed: the members of OMF are not people, but more than 40 modelling institutions; people are involved by participating in one or more of OMF's working groups.

8.5. From micro to macro: 'theories out'

The theories that we hope to develop using ABMs are not only those that explain decisions and behaviour at the agent or micro level but, equally importantly, those that explain dynamics at the system or macro level. It seems, however, that system-level theories are rarely addressed with ABM. This is in stark contrast to Dynamical Systems Modelling, which systematically explores the relationship between the feedback structure of a system and its dynamics (Radosavljevic et al., 2023). Similar analyses relating the key design features of an ABM to system-level properties, such as resilience, buffer capacity, or response to change and multiple stressors, should be possible. To date, analyses of, for example, resilience using ABM have been limited (Egli et al., 2019), again because of insufficient attention to context. System-level concepts such as resilience are multidimensional, including different stability properties (variability, recovery, resistance), reference states, state variables, disturbance types, and temporal and spatial scales as dimensions (Grimm and Wissel, 1997). These dimensions are part of the context that defines an ABM. If an ABM focuses only on a specific context, as most of the ABMs reviewed by Egli et al. (2019) do, there is not much to learn about general mechanisms and principles.

That the micro and macro levels of ACS are interrelated is well known and has been visualised using 'Coleman's boat' (Ylikoski, 2021), but we need better methods and strategies to explore this interrelationship. One approach could be to use ABM and dynamical systems models in parallel, so that the system-level perspective informs ABM design and analysis, and vice versa (Radosavljevic et al., 2024).

8.6. A vision: how to move on?

This special issue contains valuable contributions that not only document the progress that has been made but also outline the next steps that need to be taken. In addition, in this concluding section, we would like to offer a vision of what the future might look like. While we acknowledge that not all details and necessary steps are fully known, this vision is intended to inspire and guide future research and to outline a potential trajectory for further development.

ACS are unique – as the discussions in this special issue show – in that they can be conceptualised at two levels, the agent and the system level. Any search for theory or general principles must therefore address these two levels and the interplay between them. This includes the feedback between the two levels, which often shapes the evolution of ACS. Very early on, ABMs were identified as a promising method for capturing the inherent complexity and dynamics of ACSs (Huston et al., 1988). They can provide a computational testbed for investigating how ACSs function and respond to change, ideally providing predictive guidance in a changing world.

Fig. 3 illustrates our vision of how the virtual laboratory provided by ABMs can also be used to promote theory development. The starting point is identifying empirical patterns concerning the ACS of interest. These patterns provide the empirical basis for selecting appropriate theories or general principles at both the agent and the system level.

First, patterns are used to select theories at the agent level. Since agents and their behaviours are the building blocks of ACS, the development of extensively tested theories of these behaviours is crucial. We use alternative theories and compare them in terms of their ability to reproduce multiple patterns observed in reality when incorporated into the overall ABM ("pattern-oriented modelling" (Grimm et al., 2005; Wijermans et al., 2023). This corresponds to the scientific method of "strong inference" (Platt, 1964). In this process, ABMs should be seen as virtual laboratories where we can develop and test alternative theories of decision-making and other processes "in silico" (Klingert and Meyer, 2012; Lorscheid and Meyer, 2021). As a result, iterative agent-based theory development leads to models that constitute "theories of agent behaviour" (TAB), which are not intended to be perfect representations in themselves but are good enough to explain patterns observed at both the agent and system levels. This ABM theory development strategy has been proposed in ecology (Grimm and Railsback, 2012; Railsback and Harvey, 2002) and is now spreading to other disciplines, including human behaviour modelling and urban studies. This approach also allows us to address the context dependency of theories. Rather than focussing on single contexts, i.e. settings in which a theory works, it is also important to try to break the theory, i.e. to find settings in which the theory begins to fail. For this, robustness analysis is an important method; it aims to break theories and models (Grimm and Berger, 2016b).

Furthermore, we believe that simply imposing key agent behaviours makes it difficult to iteratively test, learn, and improve theories at the agent level. Such iterations require testing a TAB in new contexts, in different periods, and under new conditions. For this reason, the explicit distinction between behaviours that are imposed and those that emerge from first principles is now gaining ground in ecology. For example, the mortality of fish can be imposed by imposing a certain probability of death, or it can emerge from the choices made by the fish, e.g. habitat selection. Here, the behaviour of agents would emerge from basic principles. These are fundamental mechanisms that underlie adaptive behaviour and decision-making, focussing on the response to changing conditions. TABs based on first principles can therefore be used for a wide range of contexts and conditions without recalibration (DeAngelis and Diaz, 2019; Grimm et al., 2017; Railsback, 2001). Corresponding first principles still need to be identified for human behaviour, and will be more complex than in ecology, but there is no reason to believe that

[1] https://www.openmodelingfoundation.org/.

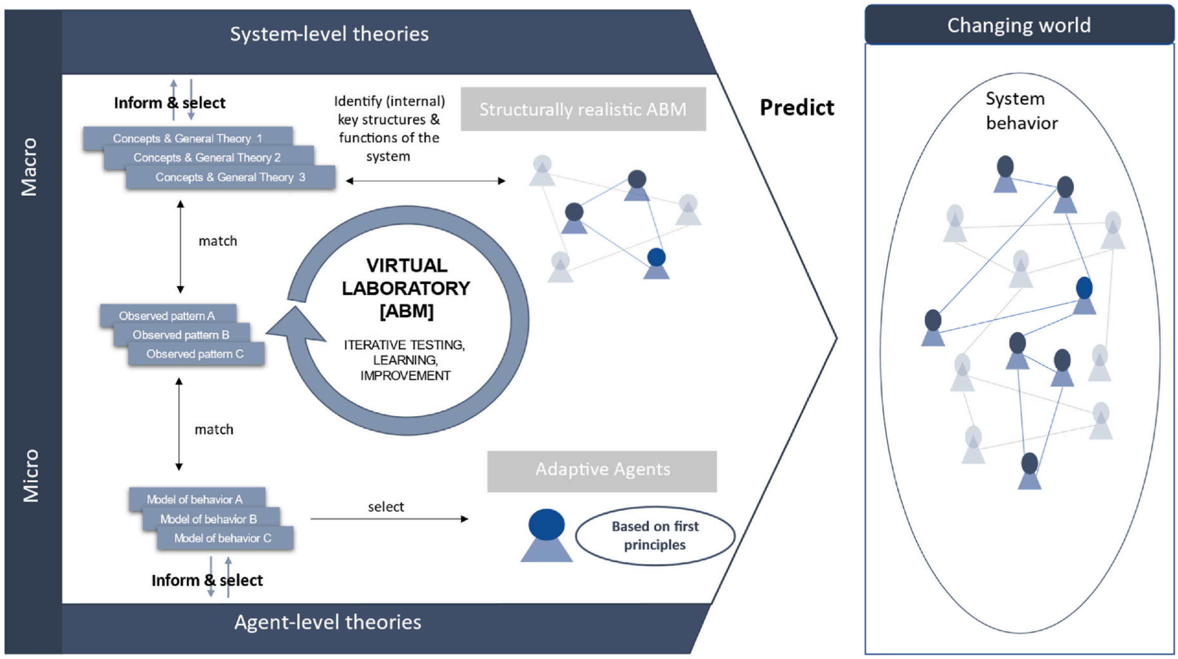

Fig. 3. To meet the challenges of our rapidly changing world, we need models that can predict the dynamics of ACS. To be useful beyond individual cases, models are ideally driven by elements and mechanisms that remain relevant as the world changes. To this end, ABMs are used as virtual laboratories for agent- and system-level theory development, based on an iterative process of theory development through testing, learning and improvement (modified from Berger et al. (2024)).

such principles may not exist.

Secondly, patterns can also inform about the system level of an ACS, i.e. they can point to the internal organisation of the system. For example, patterns of oscillations of variables may indicate negative or positive feedback loops within a system, the existence of buffers or constraints. The vision is to strive for both tested theories of agent behaviour and structurally realistic models of the internal structure of ACSs. Here, "structural realism" refers to the ability to reproduce a whole set of patterns that characterise the system for the right reasons, thereby capturing the internal organisation of the real system, rather than tweaking the model through extensive calibration (Wiegand et al., 2003).

Such structurally realistic models of ACSs are key to developing general theories of how they work. Such theories address fundamental questions about how systems persist, are organised, and function. Examples include resilience (Holling, 1973), hierarchy (O'Neill et al., 1986), and network theory (Gao et al., 2016). To move from ABMs to general system theories, two further elements are required but still largely lacking: (1) systematic analyses of how these ABMs of systems work, and (2) relating these ABMS to existing system theories. This would involve learning from other modelling approaches to complex systems, such as systems dynamics, operations research or systems biology. These fields have developed powerful strategies and metrics for identifying core mechanisms and feedback.

Systematic model analysis identifies key mechanisms that can serve as building blocks for general system theories because they are likely to be relevant across systems, for example, that local flammability in a wildfire ecosystem depends on the time since the last fire (Zinck and Grimm, 2009), that spatial patterning of host species can facilitate the eradication of wildlife diseases such as rabies (Eisinger and Thulke, 2008), or theories such as the "State-based Predictive Theory" of animal behaviour (Railsback and Harvey, 2002; Railsback and Harvey, 2020). However, there is still no established culture of trying to understand how an ABM actually works. This was criticised 25 years ago in ecology (Grimm, 1999) and more recently in the social sciences (Schulze et al., 2017), but progress is slow. It would require both a stronger focus on prediction and explanation rather than mere representation, and more systematic analyses, in particular robustness analysis (Grimm and Berger, 2016b), which means simplifying an ABM to the point where it is no longer able to reproduce the set of patterns that characterise the system.

Finally, theory development that proceeds from cases to general principles by targeting classes of systems should be possible both within and across disciplines. In economics, this vision is expressed in the concept of "stylised facts", which, as opposed to patterns observed in specific systems, refer to patterns identified for, and thus circumscribing, entire classes of systems (Meyer, 2011). For financial markets, several stylised facts, such as fat tails of asset returns, have been proposed to be characteristic of different financial markets (Hommes, 2002). Similarly, stylised facts of economic growth (Kaldor, 1961), urbanisation (Pumain and Sanders, 2013) or collusion (Heine et al., 2005) have been proposed. Similarly, in ecology, patterns or stylised facts are used to define ecosystem types. For example, savannas are defined by the coexistence of trees and grass with a maximum tree cover of about 20% (Jeltsch et al., 2000).

The identification of stylised facts may be facilitated by new techniques of pattern recognition based on machine learning. Nevertheless, the development of system theories through agent-based modelling is an approach that combines inductive and deductive elements. The development and testing of system theory can start from concrete cases, but deduction also plays an important role. Existing system theories, broad assumptions based on intuition, theories from other disciplines such as physics, or conceptualisations (such as network theory) provide roadmaps for analysing ABMs, which then allow us to explore their potential for making robust predictions about how systems will respond to changing conditions.

Realising this vision of theory development is a community effort. Collaboration in this effort across modelling projects and disciplines will be facilitated by standards for model design, communication, and analysis. However, there will be no theory if we do not strive for it.

CRediT authorship contribution statement

Volker Grimm: Conceptualization, Writing – original draft. **Uta**

Berger: Conceptualization, Writing – review & editing. **Matthias Meyer:** Conceptualization, Writing – review & editing. **Iris Lorscheid:** Conceptualization, Funding acquisition, Project administration, Writing – review & editing.

Declaration of competing interest

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

Data availability

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