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What can life cycle assessment modeling gain from agent-based modeling?

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Abstract

Integration of agent-based modeling (ABM) and life cycle assessment (LCA) has been proposed and applied as an approach to leverage the complementary strengths of both methods in assessing sustainability impacts within complex socio-technical systems. However, the existing literature has focused primarily on the technical “how” of integration, while the rationale, benefits and drawbacks have received less attention. In this forum paper, we revisit the integration of ABM and LCA from a conceptual standpoint and examine how ABM can contribute to LCA across four dimensions, namely temporality, dynamicity, scale/spatiality, and causality. We position ABM as a method for enhancing recent advances in different “flavors” of LCA, such as dynamic, prospective, territorial, and consequential approaches. We argue that an agent-based LCA approach constitutes a paradigm shift in sustainability assessment because it facilitates holistic understanding of consumption-production systems, explicit modeling of policy interventions beyond technological change, and supports decision-making under deep uncertainty, while requiring fundamentally different empirical data and validation approaches. We also offer a practical guide to support practitioners and researchers who aim to apply this interdisciplinary approach. By clarifying the rationale for integrating ABM and LCA, this article can assist and guide them in their research design and practice. In this way, this forum paper explicates the “why” underlying the use of the agent-based LCA approach, which responds to the challenges of modeling complex socio-technical systems, and ultimately advances sustainability assessment.

Keywords Agent-based modeling · Life cycle assessment · Complex systems · Socio-technical system · Sustainable consumption and production · Industrial Ecology

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1 Introduction

Anthropogenic climate change, biodiversity loss, and pollution constitute the “triple planetary crisis” (United Nations Environment Programme, 2021). These interconnected threats endanger Earth's systems and future generations. While these threats need to be addressed urgently, tackling such complex and multidimensional problems is challenging. Adopting a life-cycle perspective has been acknowledged as one approach that can help identify sustainable solutions (Hellweg et al., 2023). In this context, Life Cycle Assessment (LCA) has become one of the most commonly used methods for evaluating the sustainability impacts of products and services through the entire lifecycle, from resource extraction and use to end-of-life disposal.

However, LCA tends to focus predominantly on specific products or services, rather than on complex production-consumption systems. Furthermore, the consumption side, which inherently relies on human decision-making, generally

receives less attention (Hicks, 2022). Given the important role that human behavior plays in shaping the sustainability impacts of complex production-consumption systems, it should be considered in the design of effective sustainability policies (Nielsen et al., 2020, 2024). In response to the growing recognition of complexity in sustainability policy-making, agent-based modeling (ABM) has been identified as a promising approach for integrating human behavior and decision-making into policy design and for simulating potential consequences of interventions (Assefa et al., 2026; Baustert et al., 2025; Belfrage et al., 2024b; Castro et al., 2020; Mehdizadeh et al., 2022; Ribeiro-Rodrigues & Bor-toleto, 2024; Walzberg et al., 2023).

While ABM and LCA are two distinct approaches, the integration of ABM and LCA has been proposed and applied to leverage their unique strengths in understanding complexity and quantifying sustainability impacts (Axtell et al., 2001; Davis et al., 2009; Dijkema et al., 2015). To date, several review and perspective articles have been published regarding integration methods and degrees of coupling (Micolier et al., 2019a), uncertainty analysis in consequential modeling (Baustert & Benetto, 2017), comparative analysis of circularity assessment methods (Walzberg et al., 2021), benefits of incorporating human behavior in modeling (Hicks, 2022), and application to circular economy (Walzberg et al., 2023). However, these articles mainly focus on ABM and LCA as the subject of integration and the “*how*” of integration, that is, the technical aspects, and typically provide methodological guidance for the integration process. Regardless of the diverse purposes for integrating these two modeling paradigms, the “*why*” of integration, that is, the purpose, benefits, and drawbacks of ABM in terms of different types of LCA has not been systematically discussed.

Given this background, we revisit the advantages of integrating ABM and LCA from a conceptual and fundamental perspective. Specifically, we clarify how ABM contributes to different types of LCA, hereafter referred to as the “*flavors*” of LCA, such as dynamic, prospective, territorial, and consequential LCA, along four dimensions: temporality, dynamicity, scale/spatiality, and causality. Different LCA flavors are a product of diverse and evolving needs of researchers, decision-makers, and industry practitioners. Several studies have addressed the differences and similarities between LCA flavors (e.g. Di Bari et al., 2024; Guinée et al., 2018). Here, we take a different approach and focus on how ABM can contribute to Life Cycle Inventory (LCI) modeling of these four LCA flavors. We argue that the agent-based LCA approach constitutes a paradigm shift in sustainability assessment because it enables holistic understanding of consumption-production systems, facilitates explicit modeling of policy interventions beyond technological change, and supports decision-making under deep uncertainty. We provide a concise “*why*” integration guide to

support researchers and practitioners in adopting this interdisciplinary approach.

2 Flavors of LCA in modeling socio-technical systems

2.1 Role of LCI modeling

The LCI stage is both crucial and labor-intensive, serving as the backbone of an LCA model. Each LCA flavor is associated with a set of assumptions and LCI modeling approaches. In this section, we examine each dimension of LCA flavors and highlight its defining aspects of LCI modeling. Using the notion of flavors allows differentiation among various LCA types at a high level of abstraction, regarding temporality, dynamicity, scale/spatiality, and causality.

In the LCA community, the need for methodological innovation to overcome the limitations of existing flavors in addressing complex socio-technical systems has long been recognized (Reap et al. 2008a, Reap et al. 2008b). The integration of ABM and LCA can be viewed as such an innovation because it combines different flavors, as represented by the spheres in Fig. 1.

2.2 Temporality

Temporality refers to the point in time that the LCI model represents, or aims to represent, with respect to the intended use of the LCA results. The selection of a specific LCA timeframe is not mandated by any standard, but must be consistent with the goal and scope of the study (International Organization for Standardization, 2006). It can be either retrospective or forward-looking. Retrospective LCAs are used mainly to represent well established systems, such as mature technologies or markets, while forward-looking LCAs aim to represent emerging technologies or uncertain market conditions.

With the exception of historical LCA (Bruhn et al., 2024),¹ most LCA flavors rely on retrospective models, not by design but due to the nature of available data. This is not always a limitation, since snapshots of the past can provide good useful approximations of the future system states. To address this future uncertainty, forward-looking flavors such as ex-ante, prospective, or anticipatory LCA have been developed. The methodological distinctions among these approaches have been discussed widely in the literature,

¹ In this historical LCA study, the system was purposely modeled looking far back in time to understand the evolution of Danish consumption patterns.

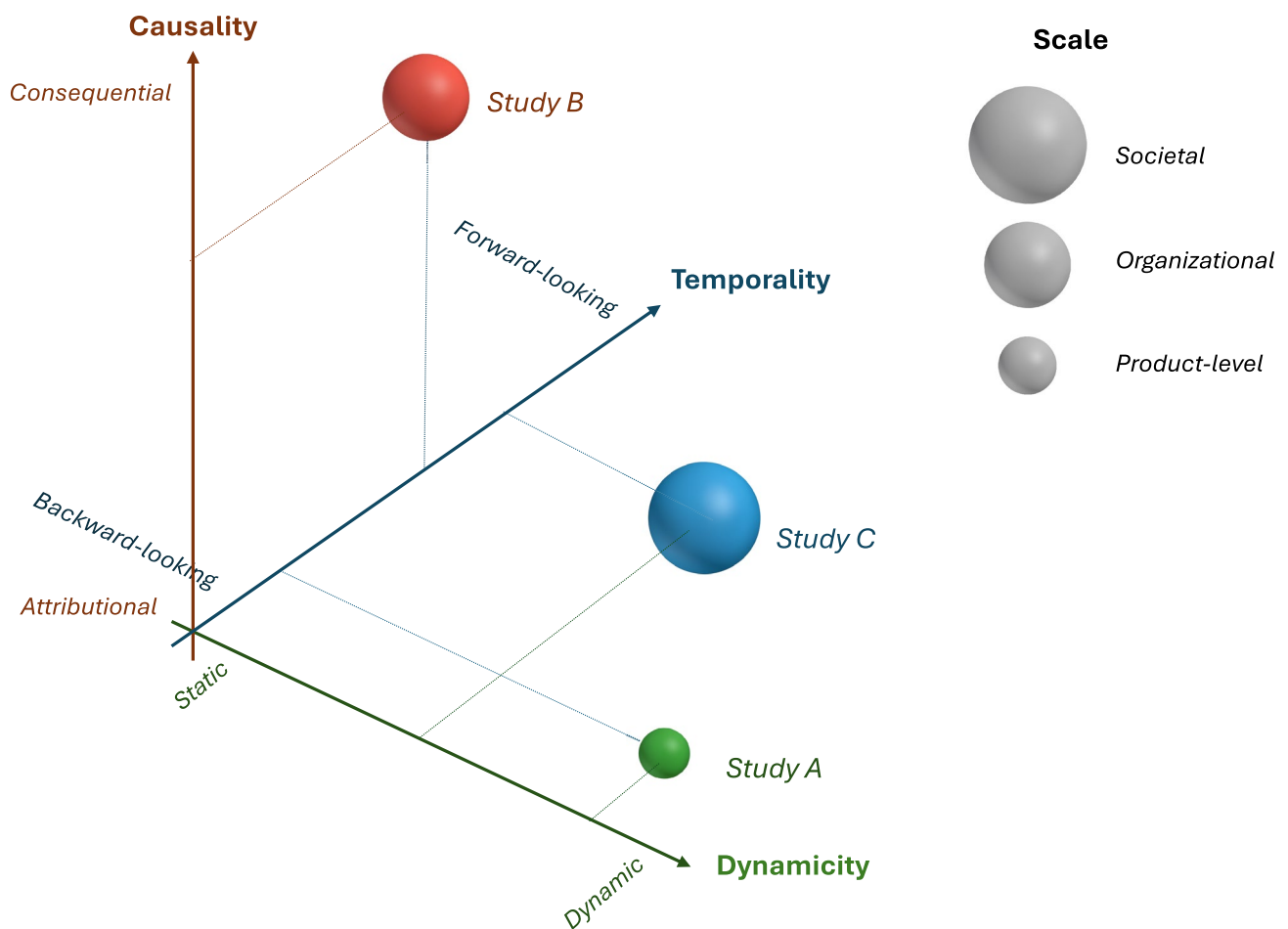


Fig. 1 Mapping different “flavors” of LCA across four dimensions. Three axes represent temporality, dynamicity, and causality, and the size of the points represents scale. LCA studies at any of the three scales may be spatially explicit. Each LCA study corresponds to a combination of one or more flavors and can therefore

be represented as a point in this space. Studies A–C are illustrative, non-exhaustive examples of LCA studies. Study A refers to an attributional, dynamic LCA focusing on a product; Study B refers to a consequential LCA focusing on a company’s footprint; and Study C refers to a territorial LCA using GIS data to analyze a region

including differences in methodology (Di Bari et al., 2024) and terminology (Arvidsson et al., 2024).

Although retrospective LCAs do not explicitly model the future state of the product system, LCA is typically forward-looking, as it is often used to provide support for current and future decision-making by companies, consumers, or policymakers regarding sustainability goals. Forward-looking flavors are currently playing an important role in policy-making, including the design of safer and more sustainable chemicals (Subramanian et al., 2023) or pathways to decarbonization (Fang et al., 2025). In these forward-looking flavors, LCI modeling extends beyond data collection to the construction of predictive approaches that anticipate possible future states. This has motivated the development of LCI models coupled with other techniques such as machine learning (Romeiko et al., 2024), integrated assessment models (Sacchi et al. 2022), and ABM (Fuortes et al., 2025).

2.3 Dynamicity

Dynamicity refers to how a system modeled in LCA changes over time. Whether examining the past or the future, the common practice in most LCA flavors is to treat the system as a static representation of reality, meaning that the background and foreground systems remain unchanged during the analysis period. In this static approach, the system is represented by a snapshot in time of production (i.e., supply chains) and consumption (i.e., goods and services markets). The LCI model is therefore simplified as an average representation of flows over a period of time. This simplification is computationally convenient because it allows the use of analytical approaches to calculate the life-cycle flows described by the LCI model (Heijungs & Suh, 2002).

However, while convenient, this practice has been criticized by several authors. They argue that steady-state models may neglect important environmental impacts that can only

be observed when a dynamic perspective is adopted (Levasseur et al., 2010). Examples include changes in supply chains and market dynamics influencing the technosphere (Abbasi & Varga, 2022), or rebound effects due to the varying vintages of energy-efficient products (Koide et al., 2022). The operationalization of dynamic approaches is far from straightforward, and in some cases requires methods beyond mainstream analytical techniques, such as graph traversal algorithms used in flavors like dynamic LCA (Pigné et al., 2020).

2.4 Scale and spatiality

Scale refers to the extent of the target system at which LCA is conducted and determines the level of aggregation of activities, flows and decision-making processes represented in the model. The LCA methodology was originally developed as a spatially and temporally independent approach for assessing sustainability impacts of various economic activities (de Haes et al., 1996). Consequently, most early LCA applications analyzed life cycle impacts at the product scale, as these were intended primarily to inform companies and consumers. This product-based scale was subsequently expanded to assess sustainability impacts at the level where decisions are being made. This led to the emergence of organizational LCA, in which an organization's full range of products, services, and activities across its operations and value chain is included (International Organization for Standardization, 2024; Martínez-Blanco et al., 2015). While organizational LCA provides a more comprehensive perspective than product-based studies, it remains limited in its ability to represent interactions across multiple actors and sectors within broader production–consumption systems.

As the scale of analysis increases—from products to organizations, cities, or regions—the level of aggregation in life cycle inventory (LCI) modeling also changes. Larger-scale LCAs typically rely on more aggregated representations of technologies and flows, but they also enable the investigation of interactions among producers, consumers, supply chains, and decision-makers. Importantly, scale in LCA should be understood as a continuum rather than a set of discrete levels. Large-scale LCI models, especially those developed with multi-regional or spatially differentiated inventories, can support analyses at multiple nested scales, from micro-level product systems to macro-level territorial units (Smetana et al., 2015; Yang et al., 2018).

While increasing the scale of LCA allows for broader system coverage, it does not, by itself, address the spatial heterogeneity of environmental pressures, resource availability, and technological configurations. To address this limitation, territorial LCA was proposed as a framework to assess the sustainability impacts of all production and consumption activities within a defined geographic area (Loiseau et al.,

2013). Territorial LCA explicitly introduces space as a modeling dimension by accounting for the localization of activities, spatial variations in environmental conditions, and the multifunctionality of land and infrastructure.

This approach is particularly relevant for supporting land-use planning and territorial governance, as it leverages tools commonly used in Geographic Information Systems (GIS) to represent spatialized inventories and impact pathways (Beaussier et al., 2022; Hiloidhari et al., 2017; Loiseau et al., 2014, 2018). As a result, territorial LCA enables a more realistic representation of how environmental impacts are distributed across space, rather than assuming spatial homogeneity.

Since its introduction, territorial LCA has been increasingly applied in domains where spatial interactions are critical, including agricultural systems (Beaussier et al., 2019; Ding & Achten, 2022), urban mobility (François et al., 2021), and waste management (Loiseau et al., 2018). At this level, LCI modeling often relies on higher spatial resolution to capture the intrinsic heterogeneity of the technosphere and its interactions with the biosphere. Territorial LCA was thus developed to support decisions at the level of territory, understood as a complex, dynamic, multifunctional, and open system in which multiple stakeholders interact to manage, use, and develop shared resources (Loiseau et al., 2013, 2018; Moine, 2006). Unlike purely scale-based expansions, territorial approaches emphasize where activities occur and how spatial relationships shape environmental outcomes, making them particularly compatible with modeling frameworks—such as ABM—that can explicitly represent localized actors and interactions.

2.5 Causality

Causality in the context of LCA refers to the cause-and-effect relationships between interventions affecting the production–consumption systems and their potential sustainability impacts. For several decades, the LCA community has debated the similarities, differences, and purposes of two flavors of LCA: attributional LCA and consequential LCA (Guinée et al., 2018). The most widely cited definition of consequential LCA is “to provide information on the environmental burdens that occur, directly or indirectly, as a consequence of a decision”, as stated in the UNEP report (Sonnemann & Vigon, 2011, page 47).² In practice,

² Attributional LCA uses a systems modeling approach in which “inputs and outputs are attributed to the functional unit of a product system by linking and/or partitioning the unit processes of the system according to a normative rule” (Sonnemann and Vigon 2011, page 132). Attribution LCA thus aims to show which part of sustainability impacts can be linked to a specific product life cycle (Guinée et al., 2018).

consequential LCA requires the LCI model to include the activities and flows expected to change with variations in demand for the functional unit (Sonnemann & Vigon, 2011). Schaubroeck et al. (2021) expanded this definition, clarifying that consequential LCA seeks to incorporate causality in LCI modeling, following the notion of Mill (1843); i.e., consequences follow associated causes in time and context, excluding other plausible causes.

Building on this logic, most LCI models in consequential LCA emphasize economic causality in addition to the biophysical and technological causality (e.g., physical flows, energy balance) represented in attributional LCA. This is commonly achieved by relying on other modeling paradigms such as economic equilibrium models, technology choice models, and system dynamics, which typically assume economic rationality in an aggregated manner (Earles & Halog, 2011; Palazzo et al., 2020).

Despite the ideal expectation of including all known causal mechanisms, constructing a fully causal LCI model is challenging. In practice, gaps in data and feasibility of modeling for various processes can make a complete and fully accurate consequential LCI very difficult to achieve. Accordingly, each study emphasizes causal mechanisms most relevant to the system under evaluation. In this sense, similar to Suh and Yang (2014), we suggest that it is more useful to describe LCI models along a spectrum of causality, rather than labelling them dichotomously. In this context, the degree of causality refers to how extensively and deeply relevant factors and their mechanisms—e.g. institutional, biophysical, technological, economic, or social—are covered within the LCI model. For example, complexity in human behaviors can exert systemic effects by altering patterns of production and consumption, which cascade through multiple sectors. Incorporating this aspect not only requires modelling materials, energy, emissions, and waste, but also requires modelling the mechanisms that describe how decisions, actions and resulting processes propagate through the system, considering dynamic feedback loops and substitution effects. Conclusively, the appropriate degree of causality to be modelled in LCI depends on the goal (e.g. explanation, prediction) of the LCA study.

3 ABM as a paradigm for LCI modeling

3.1 What is ABM?

ABM is a computational modeling approach that simulates the actions and interactions of autonomous agents within a defined environment. In contrast to LCA, which is typically solved using linear algebraic and deterministic equations, ABM involves computational simulation over time steps while accounting for the fundamental stochasticity

inherent in the system. As a methodological tool grounded in complexity science and systems thinking, ABM allows researchers and practitioners to explore how micro-level behaviors give rise to macro-level patterns, incorporating non-linearity, feedback loops, and path dependencies.

Despite advances in LCA methodology regarding incorporating temporal, spatial, and behavioral dimensions, a methodological gap remains in capturing emergent, adaptive, and decentralized phenomena. The assessment of sustainability impacts is inherently entangled with the complexity of production-consumption systems, especially when the objective of LCA is to evaluate potential transformations and dynamics within these systems. Where LCA tends to fall short, ABM offers strengths such as more nuanced behavioral rules, heterogeneity, emergence, and spatial explicitness.

One of the most important advantages of ABM is the flexibility of behavioral rules, which allows the representation of more nuanced human behaviors and social interactions (Bianchi & Squazzoni, 2015). Behavioral rules in ABM can be informed by empirical evidence and a wide range of theories, ranging from psychology and sociology, through economics and marketing, to political science (Schwarz et al., 2020; Wijermans et al., 2023). This flexibility enables moving beyond the assumption of full rationality to models in which agents, for example, have bounded rationality, are driven by social norms, or act habitually.

Another important strength is that ABM can simulate heterogeneous agents (e.g., consumers, producers, or regulators) who can learn, adapt, and interact with each other and with their environment (e.g., ecosystems). Rather than relying on representative or average agents, ABM allows the incorporation of variability in agent attributes, preferences, resource control, and decision-making processes. Including heterogeneity in ABM is essential for capturing the realism of socio-technical systems (Railsback & Grimm, 2019). Heterogeneity among agents results in diverse responses to identical conditions, making ABM particularly suitable for investigating complex interactions and feedback mechanisms. It also enables the analysis of distributional effects, inequalities, and potential unintended consequences of policy interventions.

Moreover, the ability to capture emergent properties of the system and to explore leverage points is another key advantage of ABM. This reflects the system's non-linearity and provides insight into possible evolutionary pathways (Le Page & Perrotton, 2017; Railsback & Grimm, 2019). In addition, owing to its capacity for spatial explicitness, ABM can reflect the physical context and location of agents, which influence dynamics in the system (Crooks et al., 2019).

ABM is particularly valuable in sustainability research because it can be used to explain or predict the behavior of real-world complex systems (Edmonds et al., 2019). For instance, by establishing causal chains, these models

can help identify leverage and tipping points in real-world systems. Furthermore, by allowing researchers and practitioners to simulate alternative “what if” futures and policy interventions, ABM serves as a decision-support tool that helps stakeholders to understand long-term consequences, identify leverage points, and develop robust strategies under uncertainty.

3.2 Benefits and opportunities of ABM in LCI modeling

The examples in complex socio-technical systems examined in this study demonstrate how ABM can contribute to different flavors of LCA. The integration of these two modeling paradigms, i.e., an agent-based LCA approach (Fig. 2), is not merely the addition of another flavor of LCA. Rather, it constitutes a paradigm that advances multiple LCA flavors simultaneously. Here, we discuss how ABM can support the execution of different LCA flavors.

3.2.1 ABM can yield dynamic models in forward-looking LCA

Traditional LCA approaches often struggle to capture temporal dynamics. ABM is a computational technique based on explicit time steps, and thus it is dynamic by nature. In predictive or forward-looking studies, ABM can serve as a predictive module that generates the key parameters on which an LCI model depends. Because ABM simulations are

flexible, practitioners can select short- or long-term horizons depending on the needs of the study. For example, land-use policy studies, which require long-term horizons due to the nature of land transformation, may employ annual simulation steps (Bayram et al., 2023; Ding & Achten, 2022). By contrast, studies examining human-technology interaction may use shorter time steps, such as days and even hours, particularly in analyses of occupant-building interaction (Micolier et al., 2019b) or mobility (Baustert et al., 2019). Since ABM is dynamic by default, once properly configured, any integration of ABM into LCA will produce data points annotated with their respective timestamps. This creates opportunities to combine these results with dynamic impact assessment methods (Su et al., 2017) or to incorporate tipping points and/or emission profiles into the assessment (Kaaronen & Strelkovskii, 2020). Nevertheless, this does not mean that the whole LCI model should be represented by ABM. Instead, depending on the complexity in the target systems and feasibility of modelling, ABM can be used for some specific parts (e.g., consumer behavior in use phase, stakeholder interactions in waste treatment), while other parts of LCI can be handled by a more conventional approach.

3.2.2 ABM can boost the usefulness of spatially explicit models

Conventional societal scale and spatially explicit models, such as those seen in territorial LCA, often overlook the

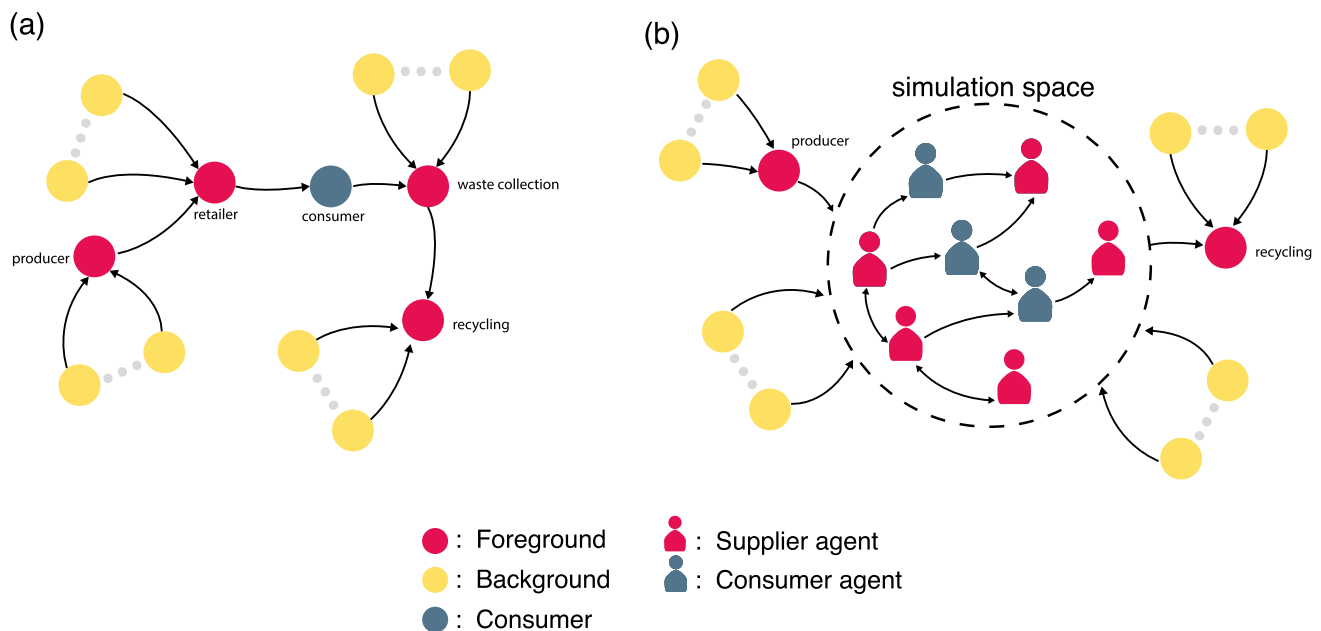


Fig. 2 Conceptual comparison of conventional LCA and agent-based LCA. **a** Conventional LCA, where products and material flows throughout the supply chain are modeled. **b** Agent-based LCA, where

the simulation space enables higher-resolution interactions among supplier and consumer agents

socio-economic behaviors of decision-makers. For example, decisions at the territorial level about land planning in agricultural landscapes (e.g., incentives) can only indirectly influence land use through farmers' reactions. Namely, in a system where farmer agents are influenced by regulator agents' decisions, how farmers' responses to planning strategies will determine the emergent land use system over time. This particular dynamic is not yet captured in territorial LCA. Moreover, given that some impact categories are location-sensitive (e.g., ecosystem quality) and depend on spatially explicit conditions (e.g., plant species in an ecoregion), integrating agents' decisions could generate spatially explicit impacts that should be accounted to better inform territorial planners (Ding & Achten, 2022).

3.2.3 ABM yields results that can be analyzed at multiple scales

ABM results can be aggregated to assign impacts to a specific functional unit. For instance, the same simulation results can be reduced to report impacts per product or per household by simply changing the point of observation. In the example of an agricultural system, environmental impacts could be allocated to a specific agricultural product (product-level), aggregated to a group of farmers (organizational), or the whole region (societal). It is important to note, however, that ABM does not eliminate the need for allocation methods, since some functional units may still require them. In case of a target product system with multiple functions, guidance for allocation to address multifunctionality in LCA could be referenced (Guinée et al., 2021).

3.2.4 ABM can help to bridge the individual behavior-systemic outcome gap

ABM results could also be linked with global top-down approaches such as multi-regional input-output (MRIO) analysis to estimate how local decision dynamics and adoption patterns ripple through global economic and environmental systems. Using ABM, planners can simulate "what-if" policy interventions (e.g., taxes, incentives, bans) and evaluate their consequences in other regions through MRIO. This facilitates comparisons of scenarios across multiple impact categories and regions, thereby bridging the gap between individual behaviors and systemic outcomes. Current territorial LCA seeks to show how decisions at the territorial level regarding land planning could influence other territories/regions (Beaussier et al., 2019). However, it remains important to assess the actual consequences to other regions when the real land-use decision makers' reactions to policy interventions are integrated.

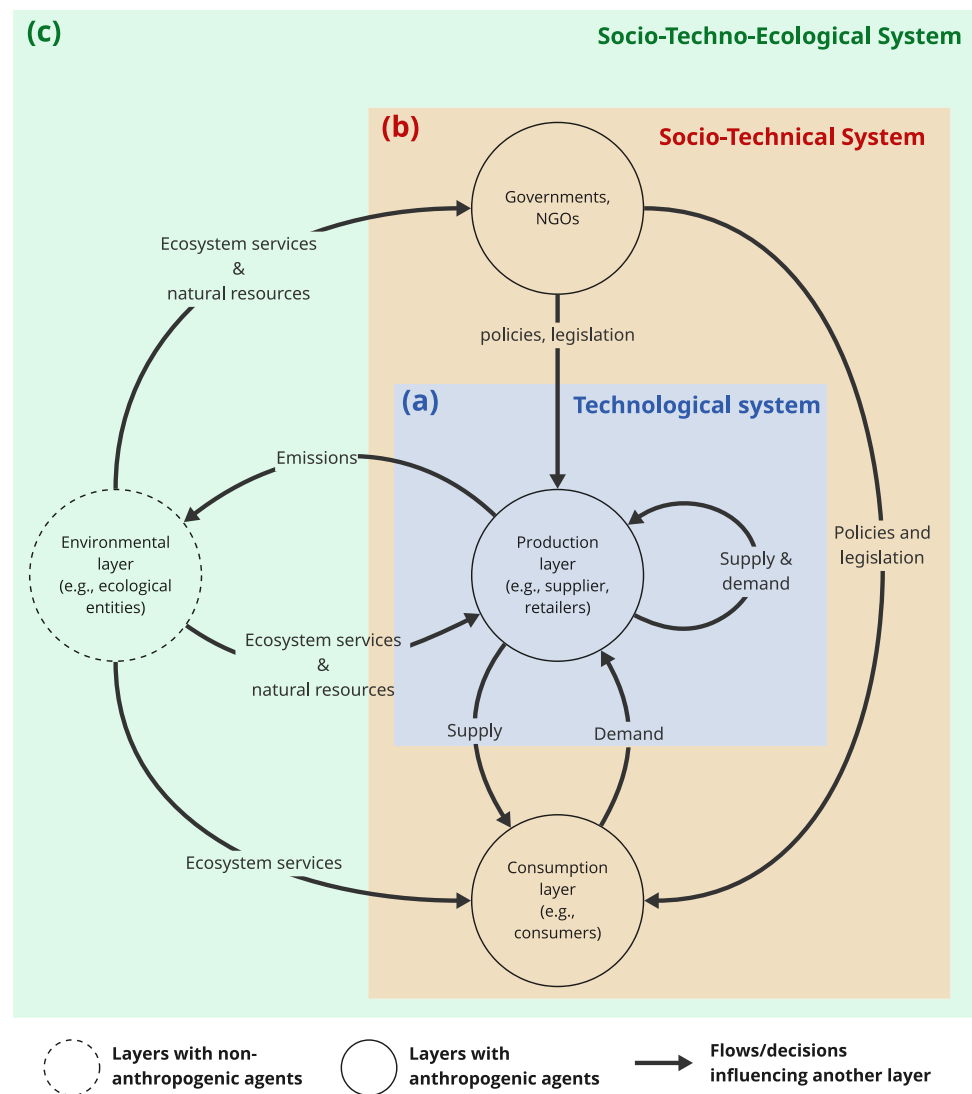
3.2.5 ABM can expand the economic rationality in consequential approaches

Existing practices of consequential LCA suffer from several limitations. For instance, economic equilibrium models assume aggregated, homogeneous market players with perfect rationality; technology choice models assume optimization decisions by industries; and system dynamics may incorporate broader social aspects, but decision-makers are aggregated without explicit representation of social networks (Palazzo et al., 2020). ABM makes it possible to model more nuanced, dynamic, heterogeneous, and interactive human behavior and decision-making that extends beyond economic rationality. For example, existing integrations of ABM and LCA incorporate social networks, habituation, environmental motivation, and diverse cognitive processes (Micolier et al., 2019a). Also, existing applications of ABM in circular economy have shown better representation of individual decision-making, heterogeneity, and externalities (Walzberg et al., 2023). Nonetheless, building nuanced and empirically grounded models is not a trivial task; it requires rigorous incorporation of social science theories in the conceptualization and formalization in ABM (Schwarz et al., 2020; Wijermans et al., 2023) and utilization of empirical data, such as statistics, surveys, interviews, and field observations (Castro et al., 2020; Ribeiro-Rodrigues & Bortoleto, 2024).

3.2.6 ABM facilitates modeling a wider range of interventions, such as public policies, business models, and physical designs

Most conventional LCA limits policy representation to technological changes (e.g., improving efficiency, switching to renewable energy), and otherwise relies on assumptions that exogenously modify technology matrices or demand vectors to represent policies through predefined scenarios (e.g., lifestyle changes leading to demand reduction). When combined with economic equilibrium models, this approach can be extended to economic instruments such as taxes and subsidies. However, the feasibility of modeling policies is fundamentally restricted by the structure of the model. In contrast, ABM's ability to capture more nuanced human behaviors allows quantification of the consequences of a wide variety of policy interventions, including economic, informational, regulatory, and other instruments (Castro et al., 2020). In this way, ABM expands policy analysis in LCA beyond technological and economic changes to encompass other drivers of decision-making.

Fig. 3 Type of systems related to production, consumption, stakeholders, and the environment. Typically, LCA focuses on **a** technological systems and treats ecological systems as externalities of inflows and outflows. An agent-based LCA can expand this scope to explicitly include **b** socio-technical systems, or **c** ecological dynamics, depending on the purpose of the specific study



4 A paradigm shift to support sustainability transition

4.1 Towards a more holistic view: integrating consumption and production sides

Much of the effort in the sustainability transition has focused on providing technical solutions and encouraging adoption in demand-side. This often results in LCA studies relying on technocratic assumptions and adopting myopic perspectives. For example, studies may emphasize the environmental benefits of electric vehicles while neglecting the social implications of mining, or highlight the low combustion emissions of biofuels while neglecting long-term land use changes. Furthermore, progress in sustainability transition has been slowed by the inertia of socio-technical systems (Markard et al., 2020; Sachs et al., 2019). Systemic changes that require shifts in consumer behavior, such as the introduction

of electric vehicles, can be culturally and politically challenging since they are shaped by social norms (Markard et al., 2020). In this regard, integrating ABM and LCA offers a more holistic paradigm, one in which sustainability challenges and potential policy interventions are assessed from a comprehensive perspective of production-consumption systems.

Nonetheless, incorporating behaviors and decision-making into the building blocks of an LCI model is not straightforward. In practice, it is not feasible to construct a comprehensive agent-based digital twin of the entire production-consumption system. This means that the selection of the system's elements to be represented as agents must depend on the practitioner's judgement. For example, when the goal is to select sustainable feedstocks for energy production, it may be appropriate to focus more on the technological aspects rather than human behaviors (i.e., physical causality) (Prasad et al., 2020). However, if a study

targets the design of circular business models, such as those observed in product-service systems for electronics (Koide et al., 2023, 2025), mobility sharing services (Diallo et al., 2023; Zare et al., 2024), urban waste sorting (Cohen et al., 2025), or industrial symbiosis (Lange et al., 2021a, 2021b), practitioners should consider the bidirectional influence of consumer and demand-side behaviors on the value chain (Fig. 3).

4.2 Endogenized modeling of policy interventions beyond technological change

ABM has been increasingly recognized as a tool for policy modeling, enabling the simulation and analysis of interventions, thereby supporting decision-makers in designing effective policies (Belfrage et al., 2024b). This is because ABM can endogenize actor's responses to policy interventions and simulate their consequences throughout socio-technical systems. This feature allows policymakers to conduct "what if" scenario experiments in a virtual setting, supporting both policy design (ex-ante) and evaluation (ex-post) (Gilbert et al., 2018).

This contrasts with conventional LCI models, in which policies are typically represented as direct changes in the technology matrix or demand vectors. In such models, the ways in which policy instruments (e.g., subsidies for research and development, guidelines for sustainable sourcing, or campaigns promoting pro-environmental behaviors) influence decision-making are not explicitly modeled but simply assumed. Studies have shown that conclusions or suggestions derived from simply adopting static or naïve up-scaling strategy can be flawed or misleading (Florent & Enrico, 2015). Flavors like consequential LCA mostly incorporate economic causality, but types of policies are still limited to economic instruments (e.g., subsidy, tax, cap and trade). Relying only on economic causality cannot account for more nuanced decision-making of organizations and individuals, critical in the adoption of new technologies (Hasan Emon, 2023). This is especially important, considering that behavioral changes involve bounded-rational, cognitive, emotional, habitual, and social factors (Gifford et al., 2011).

ABM enables researchers and practitioners to expand the range of policy instruments. The effectiveness of a policy, whether regulations, incentives, or information campaigns, depends not only on technological or economic factors but also on how people perceive, adopt, or resist changes over time (Wolf et al., 2015). ABM studies have modeled a variety of policy instruments including taxes, subsidies, trading, regulatory, information provision, and policy mixes (Castro et al., 2020). Modeling policy mixes is especially relevant given the potential for positive or negative synergies among policy instruments; for example, combining innovation

support, information provision, and economic measures can be effective for climate policy (van den Bergh et al., 2022).

To date, integration of LCA and ABM has been applied to policy analysis in various domains, including transport, building, chemical production, and agriculture (Micolier et al., 2019a). However, compared to their potential for simulating complex socio-economic dynamics, ABMs remain underutilized in policymaking due to challenges related to validation, transparency, institutional integration, and model complexity (Belfrage et al., 2024a; Castro et al., 2020). Addressing these issues through formal accreditation, post-application evaluation, and improved parameterization and calibration is essential to enhance their credibility and operational relevance.

4.3 Robust decision-making under deep uncertainty

The assessment of sustainability impacts in LCA is subject to social, temporal, dynamic, and contextual uncertainties (see the four dimensions in Fig. 1), as well as to sensitivity to model parameters. Although uncertainty and sensitivity analyses have attracted increased methodological interest, most mainstream LCA practices pay less attention to the fundamental problem of deep uncertainty about the future. Deep uncertainty reflects the pragmatic challenge of using statistical decision theory to fully capture the complexities of adaptive systems and associated challenges in decision-making. Three main sources of ambiguity are commonly identified: (i) uncertainty in probability distributions of key parameters, (ii) ambiguity in conceptual models describing system interactions, and (iii) disagreements on how to assess the desirability of outcomes (Bankes, 2002). Methodological developments in LCA have emerged to address all three sources of ambiguity; however, the extent to which they have been adequately addressed varies considerably.

Uncertainty in probability distributions is one of the main sources of uncertainty in LCA and originates from two key factors: (i) variability in LCI data, and (ii) uncertainty in background data and sustainability impact factors (Heijungs, 2024). This uncertainty has received the most attention and is dealt with in most flavors of LCA, for example, by performing extensive sensitivity analysis (Wei et al., 2015). Differently, most ABMs are intrinsically stochastic, regardless of whether the input data is deterministic or stochastic. This happens because the computation of agents' rules during runtime relies on schedulers that are commonly bound to pseudo-random generators, the hardware or the software state. Because of this, ABM typically requires multiple simulation runs with different random seeds to analyze and interpret the distribution of outcomes (Railsback & Grimm, 2019). Therefore, when LCA is coupled with ABM, uncertainty arising from the inputs and parameters for both

models, as well as the inherent stochasticity of ABM, must be accounted for when propagating uncertainty through the coupled model. Readers can consult Baustert et al. (2025) for a more comprehensive discussion and an operational framework to propagate uncertainty in coupled LCA-ABM models.

In contrast, ambiguity in conceptual models describing system interactions has been insufficiently addressed in mainstream LCA practice. As demonstrated in this paper, incorporating ABM into LCI modeling advances various LCA flavors by allowing different model structures to account for temporality, dynamicity, scale/spatiality, spatiality, and causality, whereas conventional LCA assumes a fixed linear-algebraic structure. Ultimately, the choice of model structure in LCA studies depends on the type of responsibility in which modelers and stakeholders are interested, ranging from product life cycles to the societal impacts of decisions (Weidema et al., 2018). Uncertainty in ABM and LCA coupled models propagates through multiple sources, including not only the inputs and parameters, but also model structure (e.g., functional form, choice models) and normative choices (e.g., system boundary, population size) (Baustert et al., 2025). Addressing ambiguity in conceptual models may require sensitivity and uncertainty analyses that focus on model structure rather than model parameters, leading to more careful selection and formalization of the conceptual model (Muelder & Filatova, 2018; Yoon et al., 2023).

The third source of ambiguity, the desirability of outcomes, is understudied in LCA.³ This stems from LCA's origins as a deductive, analytical school of thought focused on physical and monetary aspects. In reality, however, diverse actor perspectives can lead to disagreement on the desirability of outcomes, creating a risk of inappropriate decisions (Kwakkel et al., 2016). LCA is often used to support incremental improvements (Weidema et al., 2018), whereas real-world decision-making typically involves wicked problems (Rittel & Webber, 1973). To address wicked problems, scholars in robust decision-making under deep uncertainty (McPhail et al., 2018; Marchau et al. 2019) and adaptation pathways (Werners et al., 2021) recommend focusing on the abductive logic of possibilities and problem solving. They emphasize the central role of the actors and their sequences of actions, which can be implemented progressively

depending on future dynamics. ABM is well suited to this task because it can represent complex socio-technical systems and support the exploration of deep uncertainty that is inherent in wicked problems (Calder et al., 2018). More specifically, an agent-based LCA approach can contribute to improving our theoretical understanding, linking models with empirical data, and supporting adaptation and transformation in socio-technical systems.

ABM enables collaborative and participatory modeling, allowing stakeholders to contribute to problem formulation, data collection, problem-solving, continuous validation, and ultimately decision-making (Voinov et al. 2018). By using ABM as a decision-support system, stakeholders' opinions and knowledge can be incorporated into models to evaluate potential system changes (Étienne, 2014), e.g., addressing inequalities and unintended mechanisms and outcomes of policy interventions. We argue that integrating ABM and LCA can support decision-making under deep uncertainty; for example, as part of dynamic adaptive pathways planning, which maps the solution space over time to guide decisions under multiple types of uncertainty (Haasnoot et al., 2024).

4.4 Empirical data and validation for agent-based LCA

Empirical data and validation techniques suitable for agent-based LCA may fundamentally differ from that for conventional LCA. Although abstract ABM could be useful without empirical data for theoretical studies, empirical ABM with the use of extensive data has been increasing their roles (Laatabi et al., 2018; Zhang & Vorobeychik, 2019). Most data collection efforts for conventional LCA lie in measuring and estimating biophysical, energy, and material flows for developing foreground LCI models. On the contrary, empirically grounded ABM may require data to parameterize or calibrate the decision-making rules of stakeholders, such as consumers and producers. Collection of these data may involve methods from social sciences, including survey, interviews, field and lab experiments, stakeholder workshop, role-playing games, and census data analyses (Janssen & Ostrom, 2006; Smajgl & Barreteau, 2017). In addition, ABM can benefit from the use of big data related to the behaviors of stakeholders and products, which has become increasingly available, such as geographical and internet-based data (Crooks et al., 2017), and product-level data from digital product passport (Zhang & Seuring, 2024).

Validation in conventional LCA mainly involves ensuring quality and consistency of data, as well as independent review (European Commission Joint Research Centre Institute for Environment And Sustainability 2010). On the contrary, validation in ABM may require different approaches, especially because ABM is inherently stochastic. Over the years, scholars in the field of ABM extensively discuss how

³ The exception is methods that incorporate weighting based on social preferences, such as Environmental Footprint (EF) 3.1 (Sala et al., 2018) and LIME (Itsubo and Inaba 2003), which involves reflecting stakeholder views on weighting various impact categories into single scores. Although LCA study procedures include interpretation as a step, consideration of stakeholder values on desirability of different indicators are not typically the main focus of LCA studies themselves.

ABM validity can be improved (An et al., 2020; Railsback & Grimm, 2019; Windrum et al., 2007). ABM's variability not only arises from input parameters but also from agent interactions and emergent behaviors, resulting in cascading uncertainty from small changes in assumptions to large differences in outcomes. In addition, similar to prospective or ex-ante LCA, ABM studies often conduct forward-looking "what if" analyses. Therefore, empirical data of future status that could be directly used for validation are not available. Whenever historical empirical data is available, ABM could be validated using historic replay; in other cases, ABM may need to rely on structural validation through expert consultation and comparison with literature (van Dam et al. 2013). Validation of agent-based LCA may be challenging, but the community could learn from a diverse set of approaches and practical guidance, such as nine methods for validating agent-based models (Collins et al., 2024). Nevertheless, triangulation for validation, which involves the use of multiple data sources and methods, is often recommended. Valid conclusions require context-appropriate methods throughout all modelling stages—model design, parameter inference, uncertainty analysis, and execution. Therefore, validation of ABMs is not merely a separate step in the modelling process (Troost et al., 2023).

5 Recommendations for agent-based LCA approach

As we have shown, ABM contributes to different flavors of LCA, enabling a holistic understanding of production-consumption systems, supporting endogenized policy modeling, and enhancing robust decision-making. In this section, we provide recommendations for researchers and practitioners on how to utilize the strengths of these two methods.

1. **Why?**—Clarify why you are integrating ABM and LCA, and which flavors of LCA your approach addresses. Note that the purpose may involve one or a combination of multiple flavors (Sects. 2.1–5 and Fig. 1). Practitioners need to determine the appropriate degree of incorporating these flavors, depending on the study's objectives, familiarity with techniques, and availability of resources, since incorporating multiple flavors in LCA studies does not come without cost. Relevant guiding questions include:
 - a. **Temporality:** *Is the objective of the study prospective or retrospective?*
 - b. **Dynamicity:** *What is the time step? Does the system under study change dynamically? Are the impacts dynamic?*

- c. **Scale:** *What is the resolution of analysis? Do I want to report impacts per product unit? Should I focus on organizations or households? Am I interested in territorial impacts? How are multiple scales related?*
- d. **Spatiality:** *What is the geographical boundary? How are agents spatially embedded? How is spatial heterogeneity represented? How does the territory constrain or enable agent behavior? How does space and distance affect the agents and their interaction?*
- e. **Causality:** *Is incorporating techno-economic perspective enough and can these be represented in a causal model? Do social agents play a fundamental role in the system? Can social agents modify the system structure, scale, and dynamicity at any point? Does the study aim to support robust decision-making under deep uncertainty? Does the moment or order of decisions or interventions matter?*

It is important to make a decision to adopt or not adopt an agent-based approach, depending on the research question and characteristics of target systems. In some cases, conventional LCA can be sufficient for answering the question, but be aware that this might be due to oversimplification of the complexity in socio-technical systems. While we cannot provide a cookbook, addressing the following questions may help in deciding whether to adopt the ABM paradigm for the study:

- a. **Model purpose:** *Is the study objective to describe an existing system, or to explore possible scenarios?*
 - b. **System complexity:** *Does the system exhibit heterogeneity, nonlinear dynamics, emergent behavior, path dependence, or adaptation?*
 - c. **Social dimensions:** *Are non-technoeconomic effects relevant in the studied system?*
 - d. **Feasibility:** *Is sufficient empirical data available to model agents?*
2. **How?**—Locate your agent-based LCA modeling approach within the existing taxonomy of integration techniques (Baustert & Benetto, 2017; Fuortes et al., 2025; Micolier et al., 2019a). Be aware that ABM and LCA have different strengths and weaknesses, and consider their complementary combination carefully (Sect. 3.2). It is also important to consider feasibility of adopting ABM into LCA studies, taking into account the required resources, including expertise, computational power, and data availability (Sect. 4.4). Relevant questions include:

- a. **Direction of change:** *Do ABM results lead to changes in the LCA background system? Do LCA results provide feedback to ABM? Should the models communicate at every time step, or only at the end of the simulation?*
 - b. **Integration method:** *Is soft or tight coupling sufficient? Do you need hard coupling? Would another approach, such as surrogate modeling, be more appropriate?*
 - c. **Software:** *Which software platform should be used? Is a combination of platforms required, or is a single platform sufficient?*
 - d. **Data:** *Which empirical data is available or needed for parameterization, calibration, and validation? Which social science methods could be utilized to collect and analyze data to inform agent decisions and interactions?*
 - e. **Validation:** *Which validation techniques suit the study? Is aggregated or individual empirical data available? Are there any other methods available, such as expert consultation, literature comparison, or triangulation approach?*
3. **Which system?** — Identify the elements of the production-consumption system that contain inherent and unavoidable complexity. Be aware that the greater the number of parts of the system that are targeted, modeling more aspects of causality could be needed, requiring approaches beyond the conventional algebraic LCA. This rationale also extends to the functional unit. ABM can simulate the system as the interaction of agents, providing flexibility when setting the functional unit because it depends on the point of observation. Therefore, we suggest focusing first on system causality and then on functional unit details. Functional units in agent-based LCA can be neutral measurements (e.g., *per country, per certain number of households*) as well as conventional product-focused measurements (e.g., *kilograms, hours of product use, distance of mobility*). Due to this characteristic, different functional units can be defined for the same modeled system by adopting different points of observation. However, the choice should ultimately reflect the study's purpose, with appropriate allocation approaches applied where necessary (Sect. 3.2.3, 4.1, and Fig. 3).
 4. **Which interventions?**—Recognize that modeling the consequences of interventions beyond technological change, such as public policies, business models, and physical designs, may require an endogenized causal model of socio-technical systems, which conventional LCA treats only in a stylized way. Identify the key interventions to be modeled, consider which modeling approaches are suited to the complexity inherent in actors' responses, and justify the choice of modeling paradigm. The more emphasis is placed on behavioral and social aspects, the more complex phenomena become, which often necessitates a central role for the agent-based approach in LCI modeling (Sect. 4.2).
 5. **How uncertain?**—Acknowledge that uncertainty not only involves quantitative parameters, but also model structure (e.g., rules, assumptions, theoretical basis), which is often overlooked in some flavors of LCA. Despite the predominant reliance on linear algebraic functions in LCA, ABM allows consideration of multiple possible model structures. Researchers need to carefully select model structures and justify their choices. Where appropriate, consider conducting sensitivity analyses of alternative model structures (Sect. 4.3). Methodological and theoretical developments in robust decision-making and decision-making under deep uncertainty can provide guidance on how to address structural uncertainty (McPhail et al., 2018; Marchau et al. 2019; Haasnoot et al., 2024).
 6. **Collective knowledge**—Acknowledge that ABM, as a complexity-oriented simulation method, has challenges and limitations that are distinct from LCA, which is an empirical and data-driven method. A coordinated effort among researchers applying agent-based LCA is necessary to standardize methods, develop protocols, promote user-friendly integration techniques, and consolidate best practices for identifying appropriate methods (“how”) for each combination of purposes (“why”). Researchers and practitioners can draw on the body of knowledge and best practices established in the ABM community. This includes model documentation standards, such as the Overview, Design concepts and Details (ODD) protocol (Grimm et al., 2014) and TRAnsparent and Comprehensive Ecological modeling documentation (TRACE) (Grimm, 2020); empirical parameterization approaches, such as Data to Agent Mapping (DAMap) (Laatabi et al., 2018); frameworks for bridging social science theories and simulation, such as Modelling Human Behavior (MoHuB) (Schlüter et al., 2017; Wijermans et al., 2023); and open science platforms, such as Reusable Building Blocks (RBBs) (Berger et al., 2024) and CoMSES Model Library (Janssen et al., 2008). Similar standardized protocols or platforms dedicated for agent-based LCA could be a suitable topic for future collective efforts by this interdisciplinary research community.

6 Conclusions

In this forum paper, we offered a perspective on how ABM can contribute to conducting LCA studies of complex socio-technical systems. To this end, we mapped the landscape of LCA flavors and provided a structured perspective based on existing literature. We clarified how ABM can contribute to these flavors, which we framed as an agent-based LCA approach. This study complements existing research by clarifying and demystifying the aspects of ABM-LCA integration by adopting a more conceptual and fundamental perspective, thereby extending prior methodological contributions. Our discussion positions life cycle thinking as the overarching conceptual umbrella within which an agent-based LCA approach operates and demonstrates its relevance across the main LCA flavors. Our arguments highlight the capacity of ABM to address varying degrees of causality in LCI modeling, suggesting its suitability for inquiries such as designing and ex-ante testing of policy interventions in production-consumption systems under deep uncertainty. Acknowledging that practical implementations of agent-based LCA are far from straightforward, we provided a list of recommendations intended to support practitioners interested in adopting this modeling approach. Finally, we call for the creation of collective knowledge to facilitate the development of harmonized tools, methods, and protocols that effectively address current and future sustainability challenges. As limitations, best-practice combinations of purposes (“why”) and methods (“how”), as well as cases in which this approach is not suitable (“why not”) could not be explored in this paper and therefore represent an appropriate topic for a future review study. In this way, this position paper makes explicit the “why” of the agent-based LCA approach as a necessary response to challenges of modeling complex socio-technical systems and, ultimately, to advance sustainability assessment.

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Declarations

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