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ON THE SUSTAINABILITY OF COMPLEX SYSTEMS: UNDERSTANDING THE EFFECTS OF DISRUPTIONS IN THE SUSTAINABILITY OF SUPPLY NETWORKS

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para Julia y Augusto
para Cesar y Dayer
y para la pacha que me vio nacer

Abstract

A supply network (SN) can be broadly defined as a system with parties involved in fulfilling costumer's orders, where the essential principle is that each of them aims to maximise its profit or utility. These systems are now more complex and intertwined than ever, meaning that their modelling and assessment should include aspects of their complexity. Effects resulting from the affectation of nodes, or the SN adaptability against disruptive events hardly follow a linear fashion and can only be identified when system's evolution or companies' agency are included in the SN model. The understanding of disruptive effects, in particular, is a relevant topic since recent events have demonstrated that perturbations on SNs can propagate and generate damages to the environment and the social dimensions. While the literature has shown efforts to include complexity into methods when proposing disruption mitigation approaches, similar attempts in the field of sustainability assessment are scarce, leading to the overlook of this intrinsic SN characteristic. We argue that the strategies meant to allow the achievement of society goals, such as sustainable development, should contemplate these effects since they model systems that can show complex behaviors. We focused on determining how could we incorporate complexity characteristics into the sustainability assessment of SNs, having the study of disruptive events as an example.

We split the body of work into three parts. In the first part, we conducted a literature review in which we identified the conceptual differences between sustainability and resilience from an epistemological perspective. We identified that these concepts are decoupled from a methodological, motivational, and temporal perspective. Using these findings, we elaborated a set of four principles that should guide the proposal of any complexity-driven sustainability assessment approach. This leads to our first contribution, which is a sustainability assessment framework that is underpinned in the four principles, and that uses agent-based modelling (ABM) as main modelling paradigm.

In the second part, we dealt with the lack of flexibility and replicability of current ABM approaches that diminishes its usefulness when solving sustainability-related inquires. For this, we proposed AFRICA, a mathematical framework rooted on principles of algebraic life cycle assessment, designed to represent socio-technical agents in agent-based simulations. In addition to this, we presented the software pacha, which can perform agent-based simulations and it is designed to fit the AFRICA framework. The contribution of this part is the AFRICA framework itself because it is mathematical, flexible, and language-agnostic, so it can be implemented in any programming language.

In part three, we put to test the two previous contributions by proposing two cases of study. In the first case, we studied the effects of introducing agents with sustainable attitudes, also named Agents of Change, in a supply network. In the second case, we studied the effects that the introduction of disruptive events can have on the sustainability of the Peruvian fishmeal industry. For the first case, we demonstrated that there exist strategies and network configurations where the adoption of an environmental friendly business norm can reduce considerably the impact of the system whilst not representing a riskier decision from a financial standpoint. In the second case of study, we showed that accumulation of impacts and its trend can vary disproportionally when unexpected disruptions are introduced. Moreover, disruptions on periods of high productivity, can produce changes from which the system will hardly recover.

Finally, in this thesis, the show that the sustainability of systems under disruptive effects can be addressed by incorporating a complexity-oriented perspective into the modelling exercise. Moreover, thanks to the cases of studies, we identified two streams in which sustainability research can advance, and to which this thesis contributes. The first stream is oriented to the study of fundamental questions about the sustainability of systems, so theories, principles, or experiments can be proposed and studied. The second stream is focused on enhancing the current assessment approaches by introducing agency and dynamic components into the modelling and the sustainability assessment.

Acknowledgement

The task of listing all the individuals that have contributed, directly or indirectly, to the development of this work is complicated. Although I will make the effort to include all of those whom my fragile memory lets me recall, I apologize for overlooking on anyone. Firstly, I would like to thank my supervisor, Dr. Enrico Benetto, who during these four years has provided advisory and support in the development of this thesis and my researcher profile. His constant supervision helped me to redirect my wayward ideas, which were eventually transformed into the tangible outcomes presented in this manuscript. With his support, I reached a state in which I finally feel comfortable and motivated about the research path I have taken. This gratitude is extended to Dr. Antonino Marvuglia and Dr. Tomás Navarrete Gutiérrez, who also supervised the research project, providing meaningful contributions to its development. I want to thank Laurent Chion as well, who provided important advisory to solving coding issues during the development of the computational block. Moreover, I also acknowledge the contribution of Federico Galimberti, who during three months supported me in the exploratory data analysis. I would like to thank my colleagues of the LCSA group of the Luxembourg Institute of Science and Technology: Alex, Alya, Claudio, Elorri, Maura, Melanie, Sabina, Sébastien, Thomas G., and Thomas S. They, through discussions and lectures, nourished my views about my research and about sustainability. I also thank my friends and colleagues Ioana Popescu and Dr. Alper Bayram, who supported me in the discussion of different parts of the thesis.

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Finally, I do not want to miss extending my gratitude to the people who have been around and gave me their valuable support during this time. I want to thank my parents Julia and Augusto, and my brothers Dayer and Cesar to whom this work is dedicated to. I would also like to thank my friends Poorani, Marco, and Antonio, who became an important part of my life in Luxembourg; and to Melissa, Manuela and Renzo, who, despite being scattered around the world, managed to reach me with their affection. To Leonardo, Kevin and David, my childhood friends who, with frivolity and mischief, provided me a remembrance of home and a fresh gust of optimism in the moments of need. Finally, I would like to thank my lovely Kim, who was always with a smile on her face, and whose admirable patience I wish to gain.

Preface

My research journey started as part of a mere practicality when I tried to graduate from the university in Peru. As a civil engineer, life-cycle assessment seemed to me like such an alien application to such an alien topic: sustainability. Not much time passed until I, without noticing, steered my interests and fascination towards the complexity of the relationship among humans, our artifacts, and the environment. Since then, I have been focused on understanding how can we provide methodological improvements to our vision of sustainability through the use of computational tools. This thesis represents the natural outcome of a journey that started as an undergrad thesis and became a personal endeavour. My main motivation on writing this manuscript is to provide evidence to the reader that our current vision of sustainability can be enhanced, and that there is yet much to be done.

Gustavo Martin Larrea Gallegos
Esch-sur-Alzette, June 2024

"Imagination Is The Essence Of Discovery"
- Winston, *primate*, *scientist*

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List of Acronyms

ABM Agent Based modelling. iii, x, xi, xvii, xviii, 4, 5, 7, 8, 12, 22, 33–35, 38, 40, 42–44, 47, 54–57, 75, 76, 78, 81, 89, 106, 108–110, 112, 113, 126, 138–140, 150, 155–159,

AFRICA Algebraic Framework for RepresentIng Computational Agents. iii, x, 55–57, 59–61, 63, 65, 67–71, 73, 75, 79, 81, 88–90, 106, 109, 110, 116, 132, 149, 155, 157–159,

AIM artificial intelligence model. 32, 33,

AM analytic model. 32,

BDI belief-desire-intention. 57,

CAS Complex Adaptive System. 2–6, 15, 29, 31, 34, 37, 38, 40, 56, 108, 156, 157,

ENSO El Niño South Oscillation. 108, 109, 134,

FNR Luxembourg National Research Fund. 1,

GDP Gross Domestic Product. 108,

GHG greenhouse gases. 40, 108, 157,

LCA Life Cycle Assessment. xi, xvii–xix, 7–9, 12, 22, 24, 27, 29, 30, 34, 37, 38, 43, 54, 56, 61, 68, 75, 76, 108, 109, 112, 113, 119, 133, 140, 141, 146, 149, 150, 155, 157–159, 181, 182,

LCI Life Cycle Inventory. 34, 181,

OOP Object-Oriented Programming. 5, 110,

SAM sustainability assessment method. 15, 16, 29–31, 37, 42,

SC supply chain. xiii, 1, 2, 22–24, 26–30, 37, 39,

SM simulation model. 32, 33,

SN supply network. iii, x, xi, 1–3, 5–9, 15, 37, 54, 56, 57, 88, 89, 91, 93, 95, 106, 107, 110–112, 149–151, 155–157,

STCM Stochastic Technology-of-Choice Model. 54, 56, 182, 183,

STS Socio-Technical Systems. x, xvi, 3, 4, 10, 54, 56, 68, 69,

TCM Technology-of-Choice Model. 182,

WOS Web of Science. 17,

Chapter 1

Introduction

This chapter provides an introduction to the thesis and contains a shallow description of the topics that are treated in this manuscript. This description is meant to facilitate the understanding of the context, theory, and the cases of study presented in the following sections. The manuscript reports the progress and findings of the project AENEAS: using AgEnt based models and NEtwork analysis to assess supply chains criticalities, funded by the Luxembourg National Research Fund (FNR) (grant number: 13562095). Although the initial orientation was on supply chains' criticalities and their sustainability, the project focus shifted towards understanding complex systems and the challenge of assessing disruptions in a supply network under a sustainability assessment framework. As the reader will note throughout the whole manuscript, this turn was justified by the gaps in the literature identified in the project development. In this sense, we start by defining the key terms that are going to be used throughout the whole manuscript.

1.1 Supply networks as complex adaptive systems

1.1.1 Understanding supply systems

A supply system can be broadly defined as a system with parties that are involved in fulfilling costumers' orders, with the essential principle that each one of them aims to maximise profit or utility (Chopra & Meindl, 2007; Hassini et al., 2012). System's parties require to interact among them and the natural environment to interchange materials, money, and information. To this aim, the network of interactions can be represented to consider only direct supplier-costumer relationships (i.e., dyad), indirect relationships centred on a focal-firm (i.e., supply chain (SC)), or complete and non-focal relationships (i.e., supply network (SN)) (Miemczyk et al., 2012).

Although an SC and an SN can be topologically similar, in an SN model, nodes are not limited to represent firms, but they can also depict individuals and organizations. Moreover, these nodes are independent and can have different objectives, meaning that the system does not necessarily operate towards a common goal. The selection of the adequate level of representation depends on the adequate desired scope and objectives. Our attention is on the latter, where the system is studied in a manner that many firms and their flows are represented as nodes and edges in graphs, and the focus is on the behavior of the whole network, rather than a particular product or service. This broader representation expands the focal-firm centred SC scope in order to encompass the complexity of the system under study.

1.1.2 A definition of complex systems

The english language refers the adjective "complex" as something hard to separate, analyze or solve. Although being semantically similar, the term "complex" used in this manuscript derives from the theory used in the study of complex systems. Along the years, the study of complex systems have proposed multiple definitions that coincide in the notion of a system composed by multiple components where interaction leads to organization. In this context, Ladyman et al., 2013 proposed the following definition: *"A complex system is an ensemble of many elements which are interacting in a disordered way, resulting in robust organization and memory"*. Estrada, 2023 criticised this definition by considering it loose in indicating the nature of the interactions, which could be referred to energy, matter or information exchange. In conjunction with the "disordered" and "robust" terms, the definition is said to be imprecise because it may allow the inclusion of systems that are not considered as complex, such as crystals or minerals. Thus, Estrada, 2023 identified that the nature of the interactions in a system is key. For this and based on the work of Morin, 1977, Estrada, 2023 defines Morinian interactions as transformers of the nature of the interacting objects and of the whole formed by them. From which the following definition, which is the one considered in this manuscript, was provided:

Definition 1 *A system is said to be complex if there is a bidirectional non-separability between the identities of the parts and the identity of the whole. Then, not only the identity of the whole is determined by the constituent parts, but also the identity of the parts are determined by the whole due to the Morinian nature of their interactions (Estrada, 2023).*

A Complex Adaptive System (CAS) is a particular case of a complex system in which the system adapts itself according to exogenous or endogenous changes (Lansing, 2003; Shultz et al., 2011). When focusing on disruptions, there is still no consensual definition of the characteristics of a SN in the literature. While most studies concur in modelling the system as a graph, they treat system complexity from different perspectives (Bier et al., 2020). In this manuscript, we treat an SN as a CAS that derives from the interactions among different individuals, processes, and resources. These interactions can involve financial, product and information flows between suppliers, manufacturers, distributors, retailers, costumers (Surana et al., 2005), and even stakeholders unrelated to the value chain. Choi et al., 2001 were the first that suggested treating SN as CAS underpinned on the principles of complexity theory and analysing the intrinsic properties of an SN. They argued that an SN is emerging, self-organising, dynamic and evolving (Choi et al., 2001). In a similar fashion, Pathak et al. (2007) extended this approach arguing that a CAS is formed by agents that interact and follow simple rules, is self-organising, co-evolves with the environment, and is recursive by nature, the same way as an SN.

Moreover, this complexity can also be observed from a more empirical perspective on which we can say that an SN is complex because there is a high interconnection of nodes in the network representation (i.e., algorithmic complexity), it is difficult to set variables or equations to define the network evolution trajectory during time (i.e., deterministic complexity), and because the network behavior arises from local nodes interactions that are driven by heterogeneous motivations (i.e., aggregate complexity) (Mason et al., 2012). The interest on treating an SN as CAS rose from the necessity of understanding phenomena that cannot be easily addressed using relational models, which attempt to use variables to explain the changes in other group of variables (Pathak et al., 2007). This complexity-driven approach can be used to identify properties intrinsic to a SN, such as adaptability, robustness, resilience, or to observe the emergence of collective behaviors, such as system's sustainability.

1.1.3 The modelling of SNs

In practice, SNs are usually represented as technical networks with a predefined topology and "hard" ties (i.e., flows of materials and money) that can be addressed using analytical approaches. However, SNs are not only technological networks, but also Socio-Technical Systems (STS) where companies represent groups of individuals engaged in a productive system (i.e., technical) that interact with other companies and consumers (i.e., social). Thus, STS can be defined as a type of CAS composed by different social and technical entities that interact in a reciprocal manner (C. Davis et al., 2009; Ropohl, 1999; van Dam et al., 2013). The relationship between the different concepts presented above is depicted in Fig. 1.1.

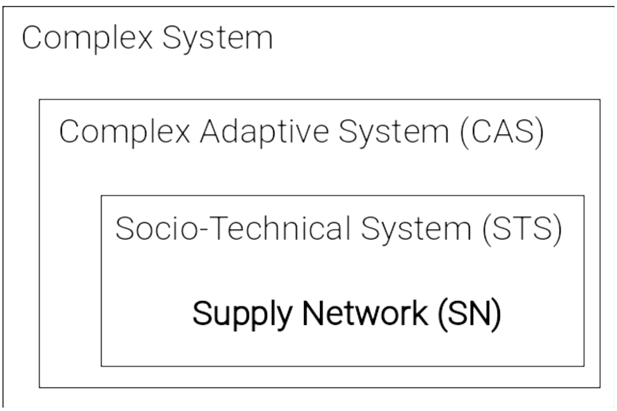


Figure 1.1: Relationship among the concepts of complex system, complex adaptive system and socio-technical system as characteristics of a supply network.

Firms' interactions are the result of decisions taken by individuals dealing with social dilemmas while being constrained by the environment and the technical state of the company or the consumer. Moreover, the importance of embracing complexity has been highlighted in literature, especially when studying the effects of disruptions (i.e., ripple and bullwhip effects), public policies (i.e., taxes and subsidies)(S. J. Davis & Caldeira, 2010), rebound effects and behavioral changes (Walzberg et al., 2019, 2020), and strategies to achieve circularity(Koide et al., 2023; Lange et al., 2022; Walzberg et al., 2023). We argue that the modelling of a STS requires and approach in which social and technical phenomena can be studied in the same modelling paradigm. In this sense, under this CAS paradigm, consumers and producers can be modeled and studied using a common and coherent approach in which inquiries related with the sustainability of the supply side, the demand side, or both combined can be addressed(Larrea-Gallegos et al., 2022).

1.1.4 Agency theory in agent-based modelling

Although it is possible to find a variety of definitions of an "agent", the framework followed in this thesis is sustained on the concepts derived from practical reasoning, the philosophical branch oriented to deal with the rationality and motivations that drive agents actions. Without the aim of presenting a philosophical discussion on the essence of practical reasoning, we elaborate on its aspects that were considered during the development of the project. There is no consensual agreement on the precise definition of an agent, however most authors coincide that autonomy is a basic characteristic (Weiss, 1999). Wooldridge and Jennings, 1995 propose a "weak notion" of agents in which they are defined as computational entities with autonomy, social abilities, reactivity and pro-activeness. However, since entities in STS represent human-like entities (i.e., individuals or collectives), it is coherent to rely on human-based notions to represent agents. Bratman, 1987 introduces the definitions of beliefs, desires and intentions as three separate and irreducible mental states. Beliefs predict the information state of the agent, while desires and intentions exert influence and control over agents' actions, respectively. These states are proper to rational agents, which can be defined as those who make decisions looking towards an objective. This rationality, as suggested by Rao and Wooldridge, 1999, implies balancing reactive and proactive behavior, balancing perception, deliberation and action, as well as balancing self-interest and community-interest.

To represent the agency of firms, the literature have adopted Agent Based modelling (ABM) as the defacto modelling paradigm because it allows to represent the system in a computational manner while acknowledging reality as a composition of autonomous and independent agents. Agents depict humans, companies or organizations and they can be considered as the fundamental and irreducible elements of the model. ABM is a bottom-up approach that permits to analyze unpredictable system properties that arise from agent's interaction rules and parameters (Nikolic & Ghorbani, 2011). Agents' rules are explicitly programmed in a computational model that simulates agents' interactions in a discrete manner.

As it was mentioned, ABM is a computational paradigm used for modelling complex systems where patterns emerge from the aggregation of agents' interactions in a bottom-up fashion, agent-by-agent and interaction-by-interaction (MacAl & North, 2010). Agents require to be explicitly programmed with particular rules that will command their actions in the simulation environment. In this sense, in an ABM, three main components can be distinguished: a set of agents, a set of relationships, and agents' environment (MacAl & North, 2010). The three components need to be explicitly programmed as part of a computational software. For this, the Object-Oriented Programming (OOP) paradigm is commonly used. In OOP, the software is an implementation of a collection of real-world objects that will interact among them when the program is executed (Garrido, 2003).

1.1.5 Disruptions and the sustainability of a SN

SN's parties require to sustain a constant interaction among them and with the environment. However, the continuity of these interactions may sometimes be affected by disruptive phenomena such as natural disasters, pandemics or alterations in the logistic operations (Kleindorfer & Saad, 2005). These unavoidable events are part of the inherent risks of supply systems (Craighead et al., 2007), and they are relevant issues to consider due to the important consequences they may have on system's functioning. Moreover, disturbances may also have effects on different aspects of sustainability (e.g., environmental impacts), especially when the operational configuration of the SN varies in order to re-adapt itself. The role of disruptions in supply systems is a subject under ongoing study that has gained more relevance, as it is reflected in the current literature (Bier et al., 2020; Katsaliaki et al., 2021). Nevertheless, the implications that these disrupted interactions may have on the environment or society are yet to be fully understood (Vlachos et al., 2019).

Studies and reviews that focus on disruption mitigation methods (Bier et al., 2020; S. Xu et al., 2020), social sustainability (D'Eusanio et al., 2019; Mani et al., 2016), or sustainable behaviors transmission (O. A. Meqdadi et al., 2019; Villena & Gioia, 2018) with a SN scope can be found in the literature. Particular aspects of a CAS, such as the aggregate complexity (Touboulic et al., 2018), or resilience (Rajesh, 2018) have also been analyzed from a SN perspective with the aim of proposing strategies to achieve sustainability. With respect to resilience, literature is extended regarding its meaning, especially because of the existence of perspectives when defining it, such as ecological, social, economic, and organisational perspectives (Ponomarov & Holcomb, 2009). In this research, we use the following definition:

Definition 2 *"Resilience is the capacity of an entity to return to an initial state after the occurrence of a disruption".*

This property is relevant in the study of CAS, and it has been constantly associated with sustainability from different perspectives. As discussed in (Bellamy et al., 2019), sustainability and SN resilience can be coupled considering resilience as a part of sustainability, sustainability as a part of resilience, or as independent concepts (Marchese et al., 2018). Studying sustainability as a whole adds another layer of complexity, especially because it requires to account material, information, and monetary flows if impacts to environment, society, and economy are meant to be calculated. Nevertheless, as presented in Larrea-Gallegos et al., 2022, the literature shows that few studies have focused on coupling sustainability and resilience for SNs in a pragmatic or quantitative way, whether it is using a life-cycle perspective (Collier et al., 2017; Pizzol, 2015), mathematical optimisation (Fahimnia & Jabbarzadeh, 2016; Hasani et al., 2021), simulation methods (Ivanov, 2018b), or paradox theory (Bellamy et al., 2019).

1.2 Motivation, research question and hypotheses

1.2.1 On the necessity of a complexity-driven sustainability assessment approach

Effects from changes on different suppliers' layers or SN adaptability against disruptive events hardly follow a linear fashion and can only be identified when system's evolution or agents' independence are included in the SN model. As a consequence, the strategies meant to allow the achievement of society goals, such as sustainable development, should contemplate these effects. In light of the absence of mainstream methodologies for assessing sustainability of systems with such CAS properties, it is relevant to identify if there is any obstacle for the development of them. Moreover, understanding existing synergies and differences among existing definitions and methods can later serve to set the basis of a sustainability assessment approach capable of integrating these concepts in a pragmatic manner. In this case, pragmatism refers to the easiness of using a modelling technique or paradigm coherent with such assessment approach. This sequence of relevant aspects can be logically depicted in a conceptual map, as presented in Fig. 1.2. Here, we can say that to understand the effects of disruptions on the sustainability of supply networks we need to rely on a complexity-driven sustainability assessment approach. At the same time, this approach requires to justify its own existence as well as to be framed by fundamental concepts. Such an approach must be operational, meaning that it should be practical and implementable as part of a methodology. Finally, we argue that with these relevant aspects covered, it will be possible to address inquiries involving sustainability and complexity.

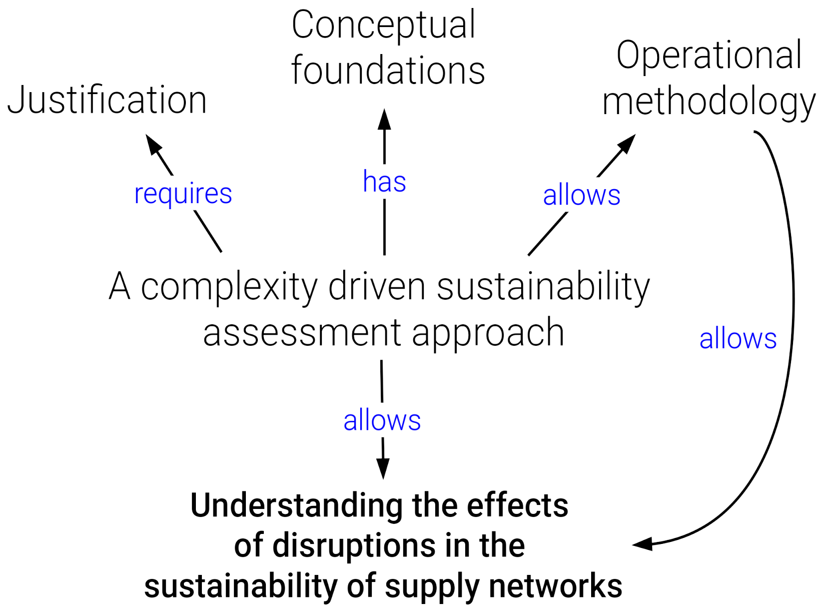


Figure 1.2: Conceptual map containing the addressed components in order to understand the effects of disruptions on the sustainability assessment of supply networks

1.2.2 Research question and hypotheses

In order to cover the relevant aspects presented in Fig. 1.2 we address the following core research question (RQ):

RQ ***How can we assess the sustainability of an SN when it is affected by disruptions?***

This RQ was extended into 4 sub RQs that will help to cover all the components of the conceptual map:

RQ 1 *How distant are concepts like sustainability and resilience from an epistemological and ontological perspective?*

RQ 2 *How can modelling objectives, such as resilience and sustainability, be coupled in the same assessment exercise in a coherent manner?*

RQ 3 *How can SNs features, such as agency, be coupled in practice with existing tools like LCA in the same operational framework?*

RQ 4 *What can the sustainability assessment of complex SNs gain from the use of behavioral information and ABM?*

In order answer of the aforementioned research questions, we have tested four hypotheses which required the development of conceptual and computational methods:

Hypothesis 1 *Sustainability and resilience are concepts interpreted differently, but they must share a common nature.*

Hypothesis 2 *Sustainability and resilience can be coupled in the same assessment exercise if such assessment approach is based on common principles.*

Hypothesis 3 *ABM can be coupled with LCA-oriented tools to model complex SNs in the same operational framework.*

Hypothesis 4 *A complexity-driven approach can provide relevant insights in addition to those already obtained with LCA-related tools.*

After a formal introduction of the characteristics of a socio-technical system in chapter 2, the manuscript addresses the RQs and hypotheses in three parts. In part I, we answer RQ 1 and 2 by deepening into the characteristics and the conceptual foundations of sustainability and resilience. We test Hypothesis 1 by studying the similarities and differences between resilience and sustainability using the findings obtained from a literature review presented in chapter 3. In chapter 4, Hypothesis 2 is tested by proposing an integrated assessment approach that relied on principles elaborated from the findings of the literature review. This part focuses on presenting the justification and theoretical foundation that are followed throughout our work. The contents of this part, including figures and tables, are in great majority our findings published in Larrea-Gallegos et al., 2022.

Part II answers RQ 3 and presents the concretion of the approached presented in chapter 4 as an operational mathematical framework (chapter 6), and a python package developed to perform ABM simulations (chapter 7). In this case, Hypothesis 3 is tested by providing an operational framework capable of coupling ABM and LCA-oriented tools.

In part III, we answer RQ 4 and we validate the utility of these framework and software by using them in two cases of study. The first case (chapter 9) explores, a fundamental question about the effects of sustainable attitudes and topological properties of an SN. The second case (chapter 10) studies the effects that variations in the availability of anchovy stock can have over the performance of a SN composed by fishmeal plants. We test Hypothesis 4 by providing relevant insights in addition to the LCA-oriented methods relying on the findings of chapters 9 and 10. Finally, we summarize and conclude our findings in part IV.

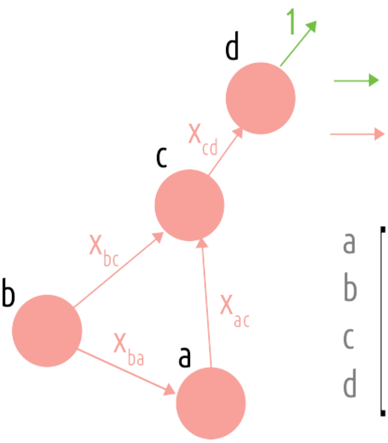
Chapter 2

From the technosphere to a socio-technical system

2.1 A graph representation of a socio-technical system

The sustainability assessment of an SN involves the analysis of system's performance considering different areas of interest (e.g., economic, social or environmental), having sustainability as a property that indicates the adequacy of a system in the basis of the "sustainable development" definition. In supply chain management, this assessment exercise is usually performed with the aim of designing or bench-marking a product (i.e., product-based). The system is modelled as an aggregation of processes and flows that are representative enough of products' manufacturing requirements that can be usually described in an analytical fashion. When assessing sustainability (e.g., environmental impacts), industrial ecology research has provided methodologies and tools to quantify sustainability-related impacts using a life-cycle perspective. In fact, production models have relied on the computational structure of Life Cycle Assessment (LCA) to account for environmental flows and impacts (Heijungs & Suh, 2002, 2006; Heijungs et al., 2013). This analytical methodology has been widely used since it provides comprehensive results, it has elegance when solving, and it is commonly used as part of a standardised framework. This preference has been strengthened due to its adequacy for assessing technological systems where flows are only constrained to established physical dependencies. Moreover, recent events have shown that SN modelling may require a less reductionist approach when complex properties are under the scope (i.e., resilience, adaptability). More specifically, situations where the system is meant to respond in an unprecedented manner (e.g, changes in policies), or to re-adapt due to unexpected events (e.g., disruptions) may need the contemplation of network's topology, agents' behaviours, and parties' heterogeneous objectives.

Modelling an SN implies building a simplified representation of the real network to fit practitioners purposes (e.g., system analysis or design). When a adopting a technological approach, a system is commonly modelled as a directed graph where nodes represent technological processes (i.e., production of an unit of product) and edges indicate flows (i.e., units of services or products). This graph is a representation of a so-called technosphere, which is defined as a system composed by all the objects created or modified by humans (Redman & Miller, 2015). When a consumer demand is imposed to a node (i.e., green arrows in Figure 2.1), it triggers a chain of demands to the rest of the nodes. In LCA, this graph is represented as an adjacency matrix (see Fig. 2.1) that is used in an accounting problem to determine, analytically, the total flows of the system given an imposed demand (Heijungs & Suh, 2002).



$$\begin{array}{c|c} & \begin{matrix} a & b & c & d \end{matrix} \\ \begin{matrix} a \\ b \\ c \\ d \end{matrix} & \begin{bmatrix} 0 & 0 & X_{ac} & 0 \\ X_{ba} & 0 & X_{bc} & 0 \\ 0 & 0 & 0 & X_{cd} \\ 0 & 0 & 0 & 0 \end{bmatrix} \end{array}$$

Figure 2.1: Technosphere graph and the corresponding adjacency matrix of the flow of goods that satisfy the demand (green arrow).

If we acknowledge that every node is a socio-technical entity, then the nodes gain an additional social layer. This layer encompasses the technical component since it is assumed that supply network's firms driven by the generation of profit and satisfying the demand. In this sense, the supply network is no longer a system of technological entities, but a system of social agents strictly constrained by a technological component. Evidently, analytic approaches cannot be used anymore because an STS cannot be depicted in just one technological matrix. In this case, determining the flows of a certain demand implies more than an accounting problem since decision dilemmas are now intrinsic to every agent. In principle, system's flows given a demand cannot be calculated in one step by solving an equation. Instead, flows can be accounted only after every agent solves its own decision and technological (if any) problems. A representation of this system transformation is visualised in Fig. 2.2. In this new graph, nodes are not entirely technological (i.e., orange), but they are embedded in a container that represents a social layer (i.e, light blue). Moreover, the direct connections between technology nodes has been overridden by social interactions (i.e., light blue arrows) since the latter rules agent's decisions. Thus, technological flows can only occur internally (e.g., technologically complex agents) or as a component of the social interaction. As it can be observed, the resulting adjacency matrix represents now a network of interactions where the edges are bidirectional because any business transaction requires, imperatively, at least two parties to occur.

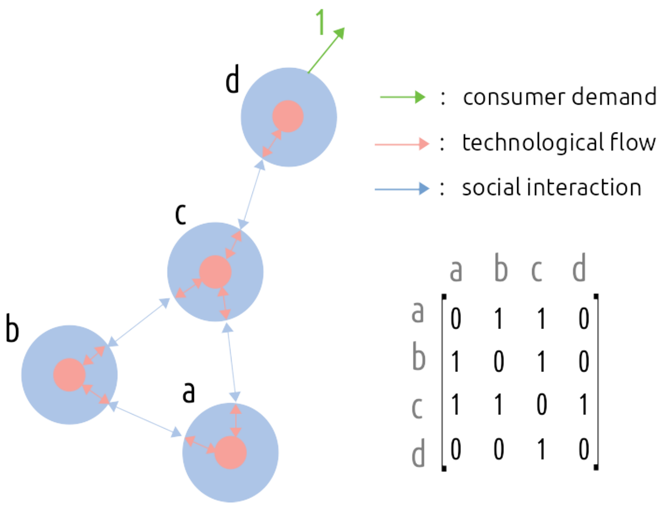


Figure 2.2: Graph of social interactions of a socio-technical system and its adjacency matrix. Orange and light blue depict technical and social components, respectively.

2.2 Agent's components and decision mechanisms

The distinction between the social and technical components does not have to be computationally explicit. Some decision aspects of companies may be based exclusively on behaviours and social networks' mechanisms, while some others may require interactions with the technical component. The degree of involvement between components depends on the context of the decision at a specific time step. For instance, agents engaged in trading with multiple suppliers can evaluate, simultaneously, physical and non-physical factors associated to themselves and to each supplier since they are leveraged by their position in the network. On the contrary, isolated agents with one or few suppliers have less leverage and their actions are reduced to maintain mere social interactions with the empowered node. In this example, node's position in the supply network has a role not only in indicating possible alternatives, but also in identifying expected agent's behaviours (Borgatti & Li, 2009).

Practitioners can use different approaches to embed these decision mechanisms in a computational method, making use of one (i.e., technological only or social only) or both components (see Fig. 2.3). In most of sustainability-oriented studies, the distinction between these two components is not explicitly made when describing the agent's rules, but they can be observed implicitly in the model implementation. The most comprehensive example can be found in C. Davis et al., 2009, in which a technosphere model was modified every time step after some nodes (i.e., agents) made decisions based on their current state (i.e., selecting suppliers). A notion of the existence of these components can also emanate when consulting literature reviews that explore the taxonomies of LCA and ABM integration (Baustert & Benetto, 2017; Micolier et al., 2019). C. Davis et al., 2009 circumvents this issue by using simulation's results to modify the values of the technosphere at every time step. In practice, the technological matrix and the algebraic representation of the system can be enhanced to consider decision factors and a formal decision mechanism compatible with the algebraic formulation of the technical system can be proposed.

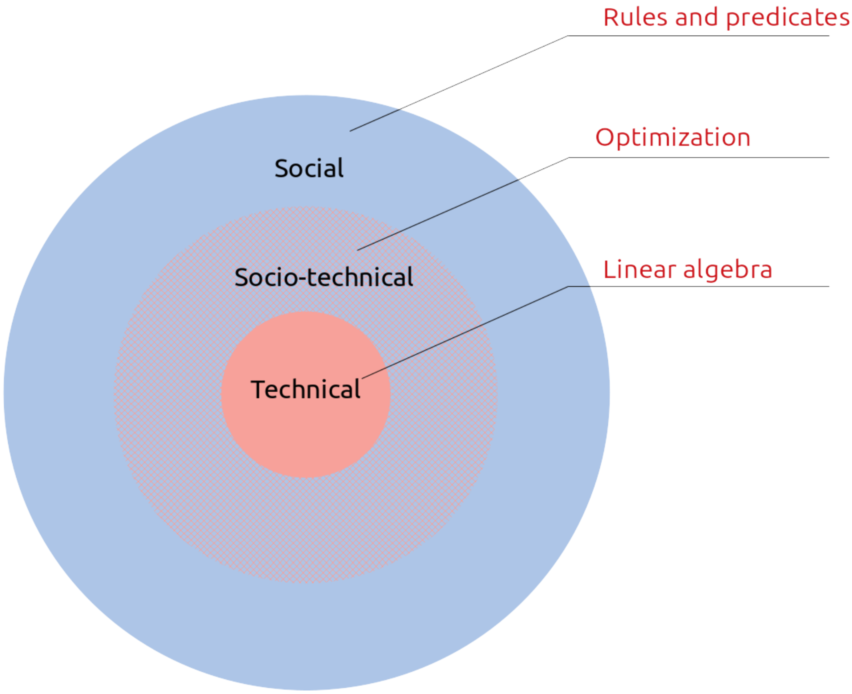


Figure 2.3: Examples of methods to calculate flows in a socio-technical system depending on the considered agent's: technosphere only (i.e., orange), social only (i.e., blue), or mixed (i.e., hashed orange)

Part I

Sustainability, resilience and complexity in supply networks: three dissociated concepts

The contents of this part, including figures and tables, are in great majority our findings presented in this publication:

1. Larrea-Gallegos, G., Benetto, E., Marvuglia, A., & Gutiérrez, T. N. (2022). Sustainability, resilience and complexity in supply networks: A literature review and a proposal for an integrated agent-based approach. *Sustainable Production and Consumption*, *30*, 946–961

Chapter 3

A non-systematic literature review

3.1 Introduction

Effects from changes on different suppliers' layers or SN adaptability against disruptive events hardly follow a linear fashion and can only be identified when system's evolution or agents' independence are included in the SN model. As a consequence, the strategies meant to allow the achievement of society goals, such as sustainable development, should contemplate these effects.

In this sense, it is important to define a conceptual framework where the development of a sustainability assessment method (SAM) underpinned by the complex nature of SNs is possible. To this purpose, we conducted a non-systematic literature review identifying the characteristics of current SAMs used for studying SN with special focus on disruptions as phenomenon of interest. We use our findings to later elaborate our conceptual proposal and to identify the requirements of the envisioned SAM. Thus, the contribution of this part is twofold: 1) it provides a comprehensive analysis of the literature linking sustainability and resilience of SN under the umbrella of complexity, and 2) it proposes a conceptual framework that can be used as a guideline to develop SAM to study complex SN.

Our critical review begins by identifying pertinent studies following the methodology shown in section 3.2. Sections 3.3.1 to 3.3.3 discuss the relation between SN structure, resilience, and sustainability, as well as dissociation and conceptual gaps. We describe the computational structure of most of SN models to later focus on complexity-oriented approaches in Section 3.3.4. In sections 4, and 4.3 we present our vision and the principles of a SAM that can embrace the nature of a CAS and a framework to be used as the foundation of a practical and quantitative method.

3.2 Methodology

Instead of focusing on a specific question or a narrow body of research (i.e., systematic review), the selected non-systematic approach allowed us to address broader and less defined questions (Cook, 2019). By using this approach, we focused on the exploration of notions and on the understanding of the literature regarding the topics of interest. In this sense, the purpose of this review orbited around two main questions:

RQ 5 *How are sustainability, disruptions and resilience treated when studying a CAS?*

RQ 6 *How do SAMs treat the complexity of a supply system in practice?*

The review consisted in the identification of relevant articles that were used to nourish the analysis and development of the conceptual framework. The scope was on articles that discussed disruptions or resilience of a SN considering a sustainability perspective, or vice-versa. In this manner, we covered the topics of sustainability, resilience, complexity and supply networks. We analysed the literature in two stages to first identify trends and a landscape (i.e., general review) and then focus our attention on our specific research objective (i.e., detailed review).

For the general review, we selected a set of keywords that described each one of these topics (see Table 3.1). While our interest was on studies with a network perspective, we also included keywords related with supply chains in the search because they were sometimes used as synonyms. The aim of this stage was to obtain a broader notion of the relationship among these descriptors. Thus, we performed search queries excluding one set of descriptors and combined the remaining in triads to create sub-queries using logic operators (i.e., AND, OR) where **supply network** was always present (e.g., ("sustainability" OR "sustainable") AND (("vulnerability" OR "criticali*") AND ("supply chain"))).

Table 3.1: List of words used for each set of selected descriptors

supply network	**resilience**	**complexity**	**sustainability**
supply chain*	resilience	complexity	lca
supply network*	disrupti*	agent-based	life cycle
	vulnerab*	agent based	life-cycle
	criticali*	topolog*	sustainab*
	robust*	complex adaptive system*	life cycle assessment
		network*	environment*
		network analysis	

We used SCOPUS database to query the articles for every combination of descriptors, considering abstracts, titles, and keywords only. The search was limited to only include journal articles published after year 2000 until March 2021. The three corpora had 11296 elements in total and resulted in a corpus of 9437 articles after merging and excluding duplicates (see DataS3 in Supplementary Material of Larrea-Gallegos et al., 2022). A terms extraction algorithm was used to obtain the most relevant 200 terms present in the corpus. The parsing and computations were performed in the CorText Manager platform (Breucker et al., 2016). Terms were ranked and selected from a trade-off between their frequency at a sentence level (i.e., frequency equals to at least 3), and their specificity (i.e.,

χ^2 score as metric of co-occurrence)[1]. After indexing the terms to every article, a terms' co-occurrence network was built and different clusters were identified using the Louvain community detection algorithm already implemented in CorTexT Manager (Blondel et al., 2008) (see Figure 3.3) (see DataS2 in Supplementary Material of Larrea-Gallegos et al., 2022).

For the second stage, we performed a more specific query using the Web of Science (WOS) database in addition to SCOPUS. For this, we made a unique query of the four topics combined to obtain articles that considered aspects of resilience, complexity, sustainability, and supply networks. The search query delivered 985 and 1071 articles for SCOPUS and WOS, respectively, that resulted in 1346 articles after merging and eliminating duplicates. These articles were later scanned by title or abstract and most of them were discarded due to impertinence or not being relevant. Moreover, due to the non-systematic nature of our review we also considered works that were not detected by any of the search queries but were still pertinent in the context of our narrative. This resulted in a total of 116 articles that were read, analysed and used to elaborate our arguments. A flowchart depicting the article identification process is shown in Fig. 3.1

[1]A more detailed description of CorTexT Manager methodology can be found in (Marvuglia et al., 2020) and in https://docs.cortext.net/lexical-extraction/

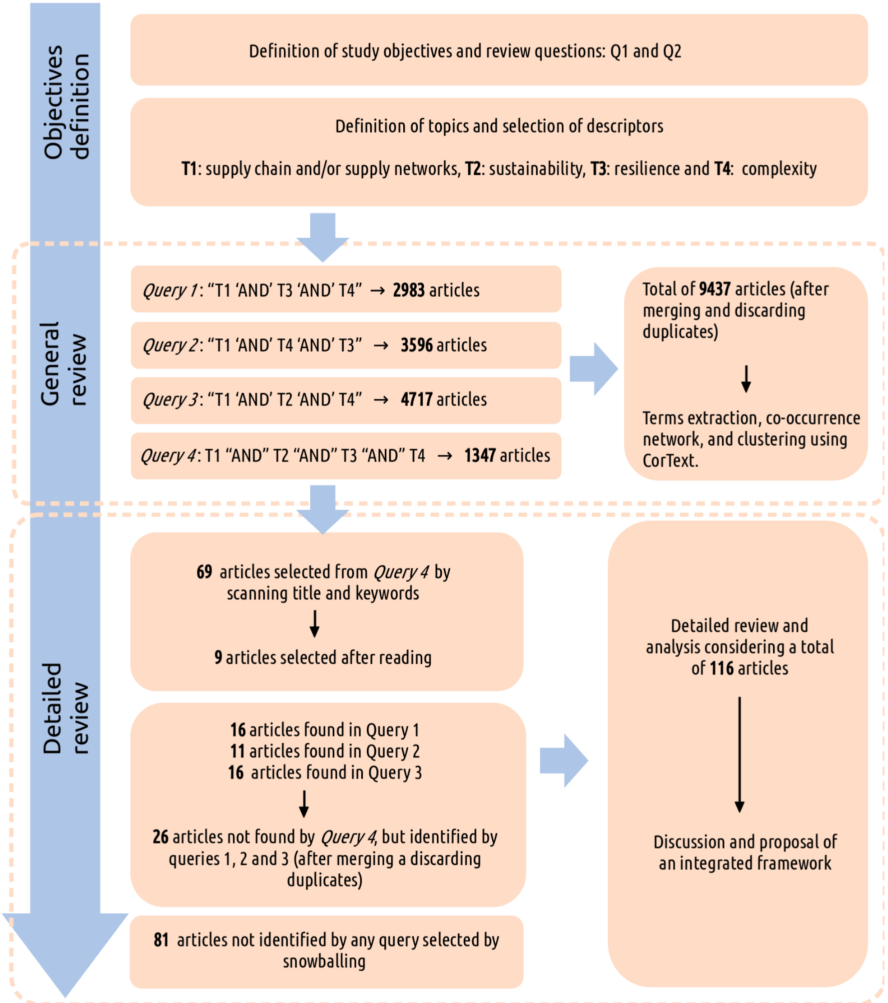


Figure 3.1: Steps followed in the different stages of the article selection process. 116 were finally selected for the literature review

We identified that most of the publications proceed from the "International Journal of Production Research" and "Journal of Cleaner Production". The rest of journals are shown in Fig. 3.2, where the category "Others" corresponds to journals with only one publication identified.

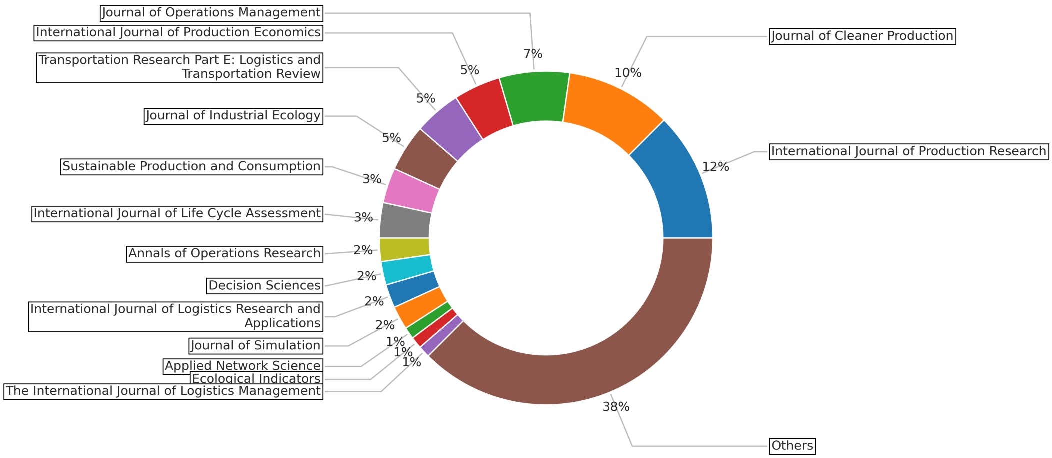


Figure 3.2: Distribution of selected articles by publishing journal. "Others" corresponds to journals with only one selected publication

3.3 Results and analysis

We used the graph in Figure 3.3 to identify distinguishable topics in literature. In the network, nodes are the extracted terms, edges indicate co-occurrence in an article, and node size represents the frequency of that term in the corpus. The resulting clusters can be interpreted as different contexts where each term belongs. As observed in Figure 3.3, cluster of terms associated with sustainability assessment methods (e.g., life cycle, climate change, environmental impacts) can be differentiated from terms related with computational methods in supply systems modelling (e.g., chain network, integer linear programming, and sensitivity analysis). This implies that these terms do not appear frequently in the same article. Moreover, it is interesting to note that terms in the disruption-related cluster (e.g., natural disasters, risk assessment, chain disruptions) are not directly connected with sustainability assessment methods terms. In fact, the only common nodes between these communities belong to the chain management cluster (e.g., case study, chain management, chain performance), which has many edges connecting disruption-related terms. While not exhaustively, this may suggest that these two areas of study (i.e., sustainability assessment and disruptions) are not abundantly related in literature.

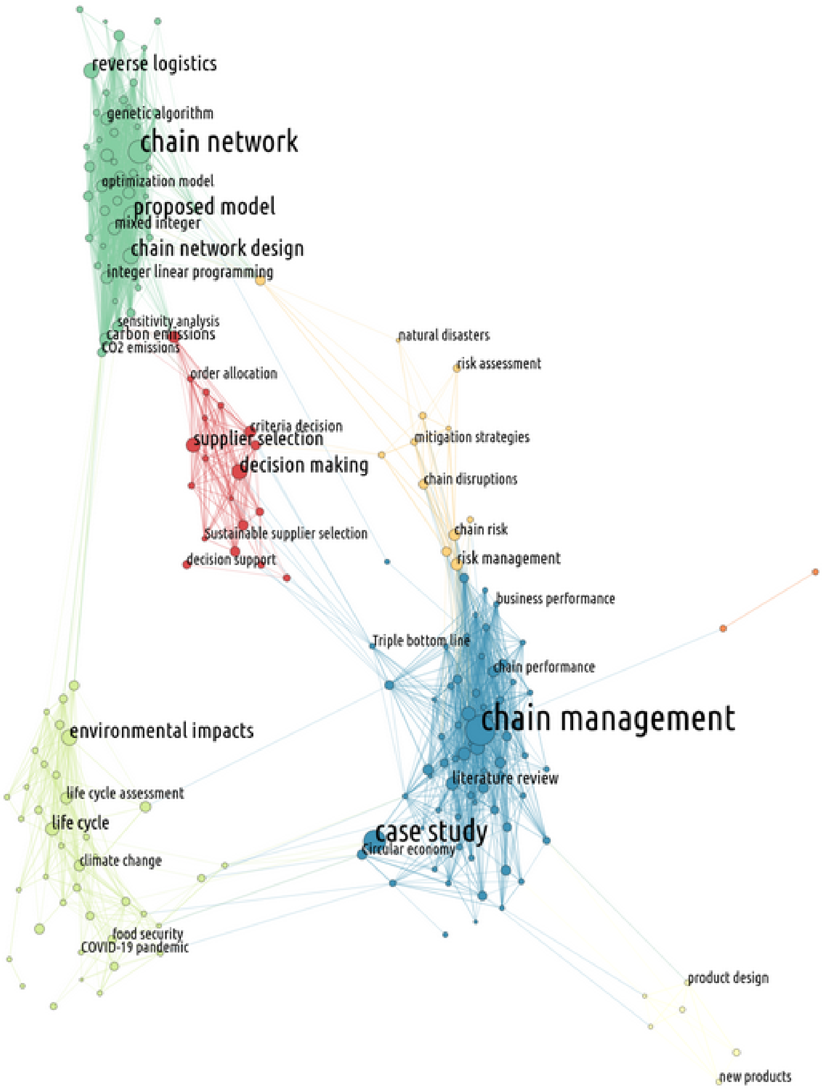


Figure 3.3: Network of co-occurrences of extracted terms in a corpus of abstracts, titles and keywords. Nodes represent terms and their size indicate the amount of times that they are found in the whole corpus. Two nodes are connected when their corresponding terms appear in the same article. Colors indicate groups that were clustered using the Louvain community detection algorithm, and they represent topics. For instance, the topic associated with sustainability-related terms (yellow) is distant from the topic related with disruptions and risk assessment (orange).

With respect to the detailed review, the scanning and abstract revision showed that only 69 articles were suited for revision considering the objectives of the study. Most of the discarded papers corresponded to articles not related to SNs, or that mentioned one of the keywords in a shallow manner. From these mapped articles, only 8 corresponded to studies that properly considered all topics of the query. In this sense, we had to include articles that were found in the general review, but did not pass the detailed review filter (See Fig. 3.1).

Compared to the articles found in the general review, this lack of publications from the detailed query depicts an absence of studies that actually cover all of the presented topics. In most of the cases, one of the terms was mentioned anecdotally in the abstract or in the keywords. Despite of this, we found that the number of publications regarding these topics has been increasing in the last years (see Figure S2 in Supplementary Material). Table 3.2 shows the characteristics of most of the selected articles and relevant examples. This classification follows the criteria later used to conduct the analysis and discussion.

Table 3.2: Relevant articles that studied SC and SN considering sustainability, disruptions or complexity

Focus	**Computational framework**	**Objectives orientation**	**Addresses complexity**	**Examples**
D/F	C	S	No	Lozano et al., 2015; Schrettle et al., 2014
SC	FL + MOO	$R \subset S$	No	Fahimnia and Jabbarzadeh, 2016; Hasani et al., 2021
SN	NA + GM	R	Yes	Arora and Ventresca, 2018
SC*	-	R + S	No	Marchese et al., 2018
SC*	-	$R \neq S$	No	Espiner et al., 2017; Rajesh, 2018
SC	LCA + MCDA	$R \neq S$	No	Collier et al., 2017
SC	LCA	$R \subset S$	No	Pizzol, 2015
SC	FL + MOO + NA	$R \subset S$	No	Zahiri et al., 2017
SN	ABM + NA	$S \subset R$	Yes	Ivanov, 2018b
SN	ABM + DA	R	Yes	Nair and Vidal, 2011
SC	ABM + NA	R	Yes	Priya Datta et al., 2007
SN	SD	$R \neq S$	Yes	Ivanov, 2020

* Review

SC: supply chain, **SN:** supply network, **D/F:** dyad/firm, **C:** conceptual , **FL:** fuzzy logic, **MOO:** multi-objective optimisation, **SD:** system dynamics, **MCDA:** multi-criteria decision analysis, **GM:** generative model, **LCA:** Life cycle assessment, **ABM:** Agent-based modelling, **NA:** network analysis ,**DA:** data analysis, **R:** resilience, **S:** sustainability

A complete description of selected articles has been shared as an excel table Data S1 in Supplementary Material of Larrea-Gallegos et al., 2022.

3.3.1 Sustainability and SN structure

We live in a constrained world, especially in terms of available natural resources, human and economic capital, and capacity of the biosphere to contain emissions and waste (Clift, 2003). In this context, the definition of sustainable development arose as meeting the needs of this generation while letting future generations satisfy their necessities (Brundtland, 2018). Among firms, the implementation of this concept has been translated into the evaluation of impacts at different dimensions such as the environment, economy, and society (J. Espinosa et al., 2019). Nevertheless, it is not unusual to find several adaptations of this concept applied to other areas. Hassini et al., 2012, for instance, define business sustainability as 'the ability to conduct a business with a long term goal of maintaining the well being of the economy, environment and society'. They introduced the definition of Sustainable Supply Chain Management as 'the management of supply chains operations, resources, information and funds in order to maximise profit, minimise environmental impact, and maximising social well-being'. Dyllick and Hockerts, 2002 define a more corporate oriented version of sustainability as "meeting the needs of a firm's direct and indirect stakeholders (e.g., shareholders, employees, clients, pressure groups and communities), without compromising its ability to meet the needs of future stakeholders as well". As it was noted, sustainability is broadly defined and it is susceptible to be interpreted in multiple ways. Because of this, firms aim to achieve sustainable outcomes by following different perspectives and strategies. In this sense, the complexity of a SN model can condition the approach adopted by the firm as well as the sustainable actions taken to fulfil the task.

At a dyadic level, implicit sustainable practices can be found during the purchasing process, which can require managers to follow codes and guidelines for selecting suppliers based on green and sustainable practices (Lozano et al., 2015; Miemczyk et al., 2012; Schrettle et al., 2014). Similarly, a buying firm can select the supplier based on its involvement in social-responsible practices, or even condition it to be involved into social initiatives (Carter & Jennings, 2002).

At a SC level, the scope is on a focal-firm and its direct and indirect suppliers and buyers. For this level, the pursuit of sustainable outcomes requires to consider firms beyond the first layer of stakeholders. Here, sustainability can be achieved not only trough an adequate selection of suppliers, but also by the incorporation of new production configurations and distribution schemes. This implies that the assessment can include stages prior to the production phase, such as material extraction, or even beyond, like the end-of-life phase. This rationale fits the fundamentals of life-cycle thinking, which consider products as sources of impacts and organisations as responsible for their own impacts and those generated throughout the product life cycle (Heiskanen, 2002). At this level, LCA is the most selected methodological framework because it can represent in a simplified manner the topology of most SC models. In many LCA studies, the SC model depicts the state of the system under average performance or stable conditions. Moreover, it allows the quantification of impacts throughout multiple layers of suppliers and life cycle phases (e.g., cradle-to-gate, or cradle-to-grave). When the target is environmentally oriented, strategies such as eco-design (Bovea & Pérez-Belis, 2012; Brezet et al., 1999; McAloone & Pigosso, 2017), environmental product declarations (Schau & Fet, 2008) and eco-labelling (Clift, 1993) are commonly evaluated. These targets can be expanded to include economic aspects, leading to the implementation of eco-efficiency (Carvalho et al., 2017; Kicherer et al., 2007) and circularity (Haupt & Zschokke, 2017) strategies.

When modelling a SC, it is usually assumed that the focal-firm has the power to influence the topology of its network to reach target goals (e.g., environmental improvement, cost reduction). Nevertheless, a firm's capacity to shape its SC decreases the more intertwined and global the network becomes (Perera et al., 2017). This aspect gains relevance when the achievement of a firm's sustainability goals relies on selecting adequate suppliers, especially because in real life these may have different motivations. The SN level expands the scope from a focal-firm oriented SC to a network of agents. At this level, a sustainable condition results from the complex interactions among the different stakeholders and it is not attributed to a firm or product, but to the whole network of stakeholders. Because sustainability is seen as a property of the system, studies focus on analysing policies, theories and firms' practices, and in understanding their effect on the sustainability of the network, rather than shaping it.

From a topological point of view, it can be noticed that a SN shall not be fundamentally different from a SC. The structure of a SC model can grow considerably until including many nodes and edges. For this, SC methods like LCA have been suited to by-pass the challenges of the resulting dense network (Peters, 2007). However, the main distinction between SC and SN models is the scope considered in the analysis. When the sustainability of the SN is pursued it is required to represent the dependency among firms in terms of decision making that cannot be directly considered using a SC a scope (Navarrete Gutiérrez et al., 2016). The SN model assumes that nodes are intelligent and autonomous, and acknowledges that the network cannot be shaped to the will of the focal firm. This change on the scope requires the use of different methodological frameworks. In this sense, the assessment approaches used to study sustainability under this scope rely mostly on qualitative (O. Meqdadi et al., 2017) and statistical methods (Villena & Gioia, 2018) to obtain insights, and computational techniques when impacts quantification is sought (Lan & Yao, 2019; Navarrete Gutiérrez et al., 2016). Many aspects of SN dynamism, resilience, network adaptation and temporal behaviors that are considered as coherent with the sustainability narrative (Anderies et al., 2013; Espiner et al., 2017) cannot be easily represented in a straight-forward manner (Pizzol, 2015). These aspects are particularly relevant in SCM when studying the SN's risk of being affected by disruptive events and its recovery capacity (Ivanov, 2020; Jüttner et al., 2003; Manuj & Mentzer, 2008).

3.3.2 Disruptions and resilience in SN

Disruptions and resilience are two concepts strictly related since the latter is a property that arises as a consequence of the risk of disruptive events. In SCM, risk can be defined as the 'expected outcome of an uncertain event' (Manuj & Mentzer, 2008), and it is commonly classified as operational or disruptive. The former refers to high-probability-low-impact events, while the latter to low-probability-high-impact events. On the one hand, operational risks are related to variations of the operation parameters during normal functioning of a system. These can lead to undesired phenomenon such as bullwhip effect, for instance, which stands for the propagation and augmentation of the high-probability-low-impact effect upstream the focal-firm (Lee et al., 1997; Metters, 1997). On the other hand, disruptive risks are associated to events that affect the functioning of the nodes in the SN. In this case, a phenomenon called ripple effect may appear and generate the downfall of the rest of the nodes downstream of the disrupted firm (Ivanov, 2018a; Scheibe & Blackhurst, 2019). Phenomena generated due to operational risks such as bullwhip effect have been widely studied in the literature (Metters, 1997), while ripple effect and disruptive risks are topics currently under study (Dolgui et al., 2018; Ivanov, 2017; Ivanov et al., 2014, 2019), especially when it refers to the environmental impacts that it may generate (Yılmaz et al., 2021).

Disruptions can be originated from different sources, such as operational contingencies (e.g., critical system malfunctioning), natural hazards (e.g., earthquakes or climate change), political instability (e.g., terrorism or economic shocks) (Kleindorfer & Saad, 2005), or global pandemics (e.g., COVID-19 pandemic) (S. Singh et al., 2020). These sources can also be denominated as drivers of risk, and they can be supplier-related (i.e., drop in supplier's capacity), costumer-related (e.g., sudden increase or drop in demand), and internal (e.g., unexpected failure at plant) (Chopra & Sodhi, 2004). Kim et al., 2015 indicate that, in many cases, disruptions do not originate from focal firm's facilities, but from nodes located along SN. They argue that disruptions at a local level do not lead, necessarily, to a network-level disruption. In this manner, SN's topology has been studied to provide insights regarding the risk of disruptions and to determine resilience of the system (Borgatti & Li, 2009; Kim et al., 2015).

Disruptive events may have tremendous impacts in the economy, environment and human life-style, but their effects can easily propagate through the different components of society. For instance, after the Great East-Japan Earthquake in 2011, the estimated indirect losses as percentage of national GDP due to disrupted supply chains were higher than the direct losses due to the earthquake (Tokui et al., 2017). In the case of the COVID-19 pandemic, the rapid contagion and severity of symptoms affected industries like apparel and food. Regarding the apparel sector, it suffered a triple hit because 1) there were direct supply disruptions, 2) the workforce was reduced due to contagions along the SC, and 3) the global demand experienced unprecedented variations (Castañeda-Navarrete et al., 2021). Similarly, reports indicate that the pandemic had an important impact in the global food industry, especially to primary producers since the initial disruptive effects reduced farming supplies and increased their prices (Béné et al., 2021).

COVID-19 pandemic is the most recent and relevant example that shows how different components of a supply system may have different paces when it refers to adapting to changes. In the case of food supply, different reports suggest that major episodes of food shortage were not observed in 2020 as it was initially expected, most likely due to primary actors coping with the disruptive effects (Béné et al., 2021). Likewise, changes downstream in consumers' behaviors (e.g., panic buy and stocking up) may generate alterations on demand that can force retailers to implement strategies to mitigate shortages (Trollman et al., 2021). In this sense, regardless of the location of the impact, disruptions will eventually have repercussions on society's well-being and adopting resilient practices becomes important.

In essence, the concept of resilience is related with the individual's ability of returning to an undisturbed condition. Nevertheless, this notion is also valid when expanding the scope to communities and organisations since it maintains its meaning (Bhamra et al., 2011). These concept has different perspectives in its conceptualisation and it has been associated with matters such as ecological and social vulnerability, the psychology of disaster recovery, and risk management (Ponomarov & Holcomb, 2009). However, when it refers to the study of SCs, it can be observed that resilience has a significant economic component, which is coherent with the main motivation of companies.

This diversity is not only present in the perspectives that conceptualise resilience, but also in the levels of practical actions that can be taken to improve it. Rose, 2004 discussed a three level view of economic resilience: microeconomic level (e.g., firms, households and organisations), mesoeconomic level (e.g., sectors or markets), and macroeconomic level (i.e., individuals and markets combined). Increasing the inventory capacity, or considering substitution of imported products are firm-oriented and belong to the microeconomic level, while setting price mechanisms, or pooling resources are sector-oriented and correspond to the mesoeconomic level. Regarding the macroeconomic level, the inclusion of individuals and organisations into the same scope generates an intertwined system where the "resilience in one sector can be greatly affected by activities related or unrelated to the resilience in another" (Rose, 2004). In this manner, the macroeconomic resilience results from the collective interaction and is not the added sum of individual actions (Rose, 2004), which can also lead to interpret resilience as an emergence property of the system. When compared with the levels of analysis of a supply system (Miemczyk et al., 2012), mentioned in chapter 1, it can be noted that the microeconomic, mesoeconomic, and macroeconomic levels are comparable to the dyad/firm, SC, and SN models, respectively. In this sense, enhancing a macroeconomic resilience would imply the consideration of a SN model.

Ponomarov and Holcomb, 2009 presented a definition that used a multidisciplinary perspective, in which resilience is defined as 'the adaptive capability of the supply chain to prepare for unexpected events, respond to disruptions, and recover from them by maintaining continuity of operations at the desired level of connectedness and control over structure and function'. Moreover, different concepts, such as robustness and flexibility, are also studied since they are aspects discussed when studying the resilience of a system. These notions, along with resilience, are associated with ideas like management strategies, self-organisation, and dependency among agents (Anderies et al., 2013). For instance, resilience and robustness are usually found as synonyms, but they describe distinct aspects of a SN's behavior. On the one hand, resilience is defined as the capacity of a system to adapt and modify its configuration without losing its functionalities. Robustness, on the other hand, is not related to the adaptation mechanism but to the capacity of the SN to withstand damage without losing its basic functionality (Perera et al., 2017). The identification and study of these aspects can be done in a theoretical or pragmatic manner. Regarding the latter, depending on the expected response mechanism to a disruptive event, resilience and robustness can be characterised using notions from graph theory and network analysis (Borgatti & Li, 2009; Kim et al., 2011), or computational approaches (Nair & Vidal, 2011; Priya Datta et al., 2007).

In this review, our focus is on understanding resilience and its integration with sustainability concepts. This is justified because a resilient network relies on the capacity of the nodes to reconnect and modify the ongoing configuration. Furthermore, as argued by Ambulkar et al., 2015, firms should learn to reconfigure their resources (e.g., adding new or shedding current) in addition to just ensuring the availability of them. From the sustainability point of view, this implies that, after a disruptive events, firms will require to select new suppliers or even modify their operational configuration in a context where sustainability-oriented policies and behaviors can influence the decision process. There are methods that aimed at integrating resilience aspects with sustainability for SC models such as LCA (Pizzol, 2015). These proxy methods are used to approach the complexity of a SN by using metrics that are representative of the structural characteristic of the network. However, they derive from static observations of the system and do not embrace the role of each node in the adaptability of the system nor the rationale behind it.

3.3.3 Sustainability and resilience: two dissociated concepts

The variety of interpretations of sustainability and resilience can be a source of confusion. Definitions used in studies might be too wide or too vague, especially when these two concepts share similar assumptions and goals, such as the aim of the system to survive (Lew et al., 2016). In essence, these concepts are akin, but in practice they address research questions following different frameworks and methodologies. This disparity is depicted in the taxonomy of combinations identified in literature reviews. Depending on the research field, sustainability and resilience objectives can be used interchangeably, treated as dissimilar, or included into one of the two (i.e., sustainability as part of resilience or vice-versa) (Espiner et al., 2017; Marchese et al., 2018). In the case of studies and disciplines that treat one concept as a component of the other, it can be observed that frameworks are oriented on identifying how can the ultimate objective of the system be achievable if one the concepts is included. For instance, studies that consider resilience as a component of sustainability evaluate how increasing system's resilience can contribute to accomplish the main goal, which in this case is to achieve system's sustainability. For instance, Karmaker et al., 2021 considers that SC sustainability can be achieved by promoting drivers that can improve properties such as agility and resilience. This logic is similar for the opposite case, where sustainability is considered as a component of resilience (Ivanov, 2018b). In the case of studies that treat these two concepts as different, it is acknowledged that they imply different objectives that may sometimes overlap, and that it is not always possible to deduct one concept from the other (Derissen et al., 2011). A more comprehensive discussion regarding the interpretation of these concepts in studies can be found in Marchese et al., 2018.

Sustainability and resilience are used to describe any kind of system, whether it is extensive as a global economy or particular as the functioning of the human body (Carpenter et al., 2001; Marchese et al., 2018). The sustainability target considered in the debate usually comes from disciplines like ecological economics, where it is linked to ecosystem services and the consequences that their affectation may have over society's well-being (Derissen et al., 2011). Nevertheless, few studies handle this discussion considering different dimensions of sustainability (e.g., impacts) (Fahimnia & Jabbarzadeh, 2016) and the complex nature of supply systems (Ivanov, 2018b). For the latter, the inclusion of complexity into the modelling exercise responds to the necessity of bringing context to the study rather than following a particular motive. Moreover, while there may exist differences in the definition of the ultimate goal (i.e., whether a resilient or a sustainable SN) (Marchese et al., 2018), it is clear that these two aspects are both valuable and important when studying and designing SNs. Indeed, we identified that mainstream methodologies for studying both of them usually converge to the same principles, but are decoupled in terms of their practical implementation. We found that this dissociation can be discussed more easily from three points of view: motivational, temporal and methodological point of view.

Motivation decoupling

In literature, SC resilience is considered as an intrinsic and structural property of the system (Arora & Ventresca, 2018; Perera et al., 2017; Shi et al., 2020; Tan et al., 2019), while sustainability is perceived as a consequent condition of the SC operation. Because resilience is oriented on SN's structure and sustainability on a desired objective, the former is usually inferred from topology, while the latter from accounting and characterising the flows. If we use eco-efficiency and redundancy as proxies of sustainability and resilience, respectively, it can be distinguished that they appear to be dichotomous measures. For instance, when the variety of suppliers of the same product is increased, the firm's productive configuration becomes more redundant, while at the same time production costs or environmental footprint may become sub-optimal and less efficient. This dilemma arises because LCA-based eco-efficiency methods envision sustainability as the main goal and they are not suited to explicitly account for system's resilience. Instead, they focus on measuring the intensity of flows rather than the structure resulting from firms interactions (Pizzol, 2015). Under a SC scope, the interpretation of both concepts and the establishment of goals is constrained to the eyes of the focal company, which accentuates this duality. An attempt to integrate resilience objectives into the sustainability goal was published by Fahimnia and Jabbarzadeh, 2016, who used an optimisation approach to include different disruption scenarios where the expected SC cost, environmental and social performance where considered as optimisation targets. In this situation, managers will aim to maximise environmental performance and reduce disruption related costs, meaning that the only solution is to find trade-offs between both aspects.

Temporal decoupling

In CAS-oriented models, the study of disruptions usually relies on simulation methods. The resilient condition of a system is determined after observing the dynamism and adaptability of simulations of the SN in a period of time after the introduction of a disruption (Y. Li & Zobel, 2020; Nair & Vidal, 2011). Even when the analysis depends on the use of proxy network analysis metrics (Tan et al., 2019), or statistical approaches (Arora & Ventresca, 2018), the aim is to understand system's resilience acknowledging that the topology may change during time. On the contrary, most of SAM usually consider a snapshot of a SC model and use its impact over certain dimensions (e.g, environmental, social or economical) as proxies of sustainability. This snapshot is made with the average configuration of the network for a given period, despite the possibility of it of being a very dynamic system. This temporal stagnation does not usually represent an issue for many environmental impacts because most of them consider a long-term span in their evaluation (e.g., climate change). Nevertheless, some other social (i.e., job losses), economic and environmental (i.e., water consumption) impacts are relevant in the short-term and, if ignored, may have negative consequences to society. The negative short-term effects that are generated after disruptive events provide the main justification for seeking more resilient systems. Integrating both concepts into a temporally flexible framework would require to encompass the system structure during a whole time span (i.e., network evolution) and to acknowledge the different affectations under different temporal horizons (i.e., short- and long-term effects).

Methodological decoupling

As explained in Section 3.3.1, sustainability is commonly studied with methods that are based on analytic approaches, such as LCA. This method, which relies on linear algebra, has the adequate computational framework to account for the system's flows required to manufacture a given product. The environmental impacts are calculated on the basis of the resources extraction and emissions from and to the environment, respectively. This SAM is SC-oriented and assumes that all agents are going to satisfy the demand, depicts the system in a stable or average situation, and mainly focuses on the flow of products or money. By contrast, methods that aim to understand or quantify SN resilience not only rely on analytic approaches, but mostly on heuristics or computational techniques as core elements of their frameworks (Ribeiro et al., n.d.). For instance, proxy methods based on graph theory not only focus on system's flows, but on network structure and its topological properties. Here, resilience is determined following heuristics that rely on network indicators that are calculated with the use of algorithms (Y. Li & Zobel, 2020; M. Xu et al., 2019). In simulations, resilience is evaluated after observing SN's behavior in a computational environment following the introduction of a disruption (Ivanov, 2017). Some LCA studies incorporate resilience aspects into the evaluation by modelling resilient scenarios (Pizzol, 2015), or by discussing scenarios using multi-criteria decision analysis (Collier et al., 2017). In studies that integrate these two concepts, we observe that sustainability and resilience are determined using different methodological assumptions and they are later integrated into a common assessment framework. Most of the studies use multi-objective optimisation methods and they represent the resilience target with proxy objective functions. For instance, Hasani et al., 2021's optimisation model considered the maximisation of geographical dispersion of SC facilities as a positive indicator of resilience against disruptions. In a similar way, Fahimnia and Jabbarzadeh, 2016 introduced disruptions in an explicit manner as scenarios in a multi-objective optimisation framework. While there were not exact measurements of resilience, this property was embedded in the sustainability goal where the system was expected to be sustainable under business-as-usual and disruptive conditions. Finally, Zahiri et al., 2017 developed a mathematical model that minimised costs, environmental and non-resilient aspects of the network. Indicators such as node complexity and demand dissatisfaction were used as proxies of resilience, assuming that they reflected how the system may respond under disruptions. In these cases, resilience was incorporated as an additional and distinct objective that required the use of optimisation techniques to allow a common framework to analyse both aspects.

Motivational and temporal decoupling condition practitioners to select different methodological pathways (i.e., methodological decoupling) when studying supply system and disruptive events. We argue that these issues can be confronted by finding a common conceptual ground that shall lead to similar objectives and to a coherent methodology. When dealing with SNs, this aspect is more relevant because no CAS-oriented framework or implementation that deal with this two concepts has been identified. In this sense, it is important to understand the computational capabilities of current modelling techniques to then select an adequate method to be set as the core of a common assessment framework. We argue that any selected computational tool should be able to contemplate the characteristics of a SN, which implies embedding the CAS nature of the modelled system.

3.3.4 Computational structure of SN models

A CAS-oriented scope embraces the notion of adaptability of the network. Moreover, it leads to a common ground where both resilience and sustainability are not determined or calculated prior any event, but they need to be observed as emergent characteristics. These characteristics need to be tangible and measurable, for instance, practitioners should be allowed to observe the constant change in topology or in sustainability metrics in the SN model. When treated as a CAS, the sustainability state is observed during the same period of time as the disruption occurs. Moreover, because the initial and final state of the system are observed, more attention can be provided to those impacts that may be brief but with significant effects. This example shows the necessity of identifying an appropriate methodology to be set as a core tool for a SAM. In this sense, we explored current supply systems modelling techniques identified in the literature to later focus on the most suitable for our goal.

Current computational frameworks

Studies aim to identify the correct configuration that allows the flow of materials or information in a beneficial way. Planning involves beginning an endeavour of re-designing a SN. The taxonomy of models is not formally defined in literature, but we are basing ours on the classification proposed by Giannoccaro and Pontrandolfo, 2001, which fits most of the studies found in literature, as stated in Peidro et al., 2009 (see Figure 3.4).

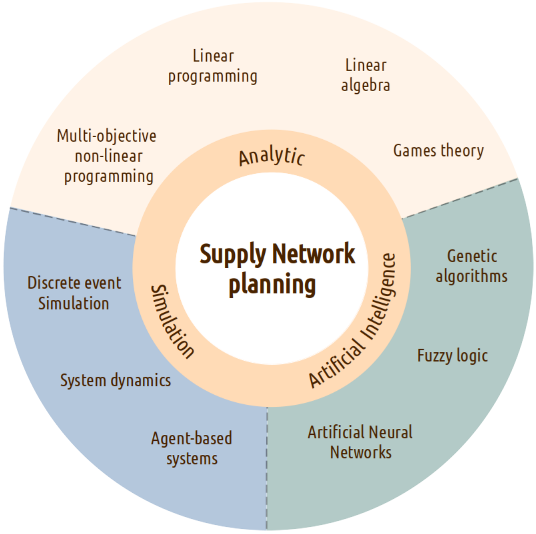


Figure 3.4: Taxonomy of modelling approaches for treating supply network planning, based on Giannoccaro and Pontrandolfo, 2001

In this sense, a SN can be analysed using an analytic model (AM), an artificial intelligence model (AIM), or a simulation model (SM). AM use linear algebra, linear programming, games theory, and all the variants of mathematical optimisation methods. They use deterministic principles to model a SN usually seeking for the optimal configuration in terms of logistic, production, or environmental impacts (Eskandarpour et al., 2015; Fahimnia et al., 2013; Ferrio & Wassick, 2008; Hasani et al., 2021; Mota et al., 2015). In the literature, studies that use AM are the most abundant, but in recent years an increase in SM and AIM has been observed (see Figure 3.5 [2]).

[2]This figure was elaborated using the extracted terms related with the taxonomy and the indexed articles identified in the *general review*

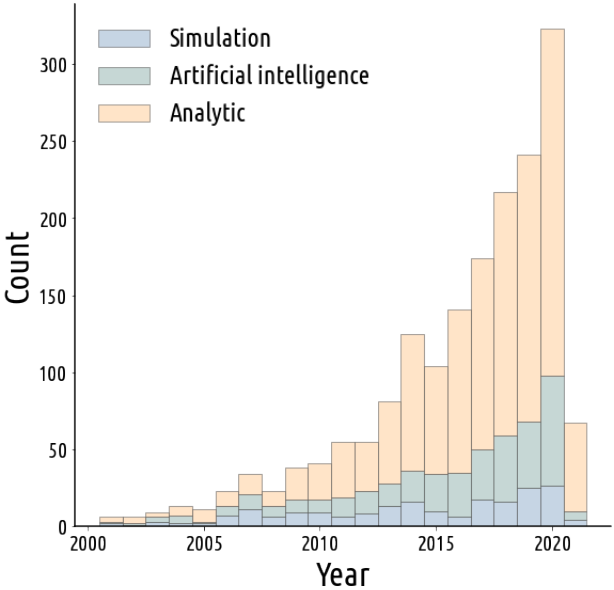


Figure 3.5: Temporal distribution of selected articles following the taxonomy of modelling approaches, based on Giannoccaro and Pontrandolfo, 2001

AIM and SM are models that use heuristics and algorithms to recreate the conditions of the SN. AIM rely on artificial intelligence algorithms and techniques such as reinforcement learning, genetic algorithms and fuzzy logic. For instance, Park et al., 2007 implemented a genetic algorithm for the planning of a SN. In Nezamoddini et al., 2020 a framework that integrated a genetic algorithm and neural networks was proposed to determine the adequate configuration of a SC. With respect to SM, these methods involve the computational recreation of the functioning of the SN in discrete steps, such as discrete-event simulation (DES), dynamic system simulation, and ABM [3]. DES is the most used and it proposes modelling systems where queues and flows are relevant and where events happen in a discrete manner. In DES, it is required to provide information regarding the logic rules that allow the flows through the whole system. ABM, on the other hand, differs from other simulation techniques because the system behavior is not modelled a priori, but it emerges after observing the simulation (Siebers et al., 2010). As explained in chapter 1, this modelling paradigm allows the simulation of agent's interactions (i.e., individuals or organisations) and conclusions regarding the system functioning are drawn from analysing the final landscape (Brandon et al., 2018). Because of these features, ABM is usually

[3] While Giannoccaro and Pontrandolfo, 2001 considers ABM as an AIM, we will refer it mostly as a SM because it has characteristics also proper that type of modelling.

selected as the modelling tool when a CAS-oriented analysis is sought (Mason et al., 2012; Pathak et al., 2007).

An ABM can be programmed to be as sophisticated as computational resources allow for. This implies that, in theory, it can be integrated with other methodologies. When it refers to sustainability, for instance, ABM simulations and LCA calculations can be integrated in the same computational framework. The degree of integration depends on the expected outcome and different classifications can be found in the literature. For example, Baustert and Benetto, 2017 classify the integration as unidirectional coupling and LCA/ABM symbiosis. A symbiosis occurs if, during run-time, LCA calculations have an effect on the ABM agents or environment, and the ABM results can influence the next step of the LCA calculations. When the ABM results feed an LCA framework, or vice-versa, the integration is considered unidirectional. Conversely, (Micolier et al., 2019) proposed a taxonomy using the terms soft-, tight- and hard-coupling. The first two refer to cases where ABM results are used to perform LCA at the end of the whole simulation (i.e., soft-coupling) or at each time step (i.e., tight-coupling). Hard-coupling, similar to LCA/ABM symbiosis, implies the mutual influence of methodologies during run time.

Regardless the type of integration, literature shows that the use of ABM allowed to enhance studies that had a limited computational framework. For instance, Navarrete Gutiérrez et al., 2015 developed an ABM in a case of the study that had previously been analysed using econometric and non-linear programming techniques. The ABM allowed them to model behaviors and interactions among farmers in maize production that could not have been represented with an analytic approach. S. R. Wu et al., 2017 argued that ABM allowed them to include human behaviors in the construction of the Life Cycle Inventory (LCI), which is a relevant aspect when analysing the building industry. Another example can be found in C. Davis et al., 2009, who proposed a soft-coupled framework that was used to understand the environmental impacts of an evolving SN (i.e., bio-electricity production), where LCA computations were performed at every time step to assess the Global Warning Potential of the electricity mix. In this sense, it can be noted that ABM has been successfully used to deliver consistent foreground data during the construction of LCI (Marvuglia et al., 2018).

As mentioned in Section 3.3.1, achieving a sustainable supply chain can have different meanings depending on the perspective of the stakeholder formulating the question (Miemczyk et al., 2012). When modelling an ABM, this conundrum is transferred to the agents when the assessment tools are integrated into the ontology of the agents. Because of this, it is important to consider the particular interpretation of sustainability that every agent might have (e.g., firm managers, producers, costumers), especially because practitioners may feel lured to impose their vision of sustainability during modelling. Sustainable purchasing behaviors, for instance, have been previously introduced in ABM whether as individual motivations (e.g., green-consciousness) (Navarrete Gutiérrez et al., 2015) or as the result of imposed policies (e.g., carbon-taxes) (C. Davis et al., 2009). Risks and disruptions can also have an influence on the decision making process of every agent, whether is directly or in a subtle manner. In a SN, disruptions have direct influence on firms' decisions, as well as the structural position of a firm may affect other companies' perceptions regarding its risk (J. Wu & Birge, 2014). In this sense, ABM can be used to understand behaviors like trust and risk propagation through the SN to increase the resilience of the system (Hou et al., 2018). Moreover, other phenomena studied in SCM, such as criticality identification, and supply and demand mismatches can also be analysed by using ABM as SN modelling framework (Huber et al., 2019; Yazan & Fraccascia, 2020). In all the cases, neither sustainability nor resilience are measured by observing an individual, but by assessing the performance of the overall system. This characteristic principle of complex systems leads to the dilemma of classifying sustainability and resilience as individual or collective properties.

ABM models were developed on the basis of the requirements of distinct resilience or sustainability assessment methods. There is still no evidence of an ABM implementation that integrates both notions from the conceptual foundations until the practical use of its outcomes. The construction of the ABM is flexible, but it requires a clear definition of the complex phenomenon that is under analysis. For this, it is important to define the ultimate research goal that will lead the modelling exercise. In this sense, we argue that a computational framework that integrates resilience and sustainability should be built underpinned by a robust and coherent conceptual framework.

Chapter 4

A complexity-driven sustainability assessment approach

4.1 Introduction

While the study of disruptions is leaning towards frameworks that contemplate SN complexity, most of SAM approaches still rely on SC models and analytic frameworks to describe topology and to derive quantitative proxies of sustainability (i.e., impacts). These approaches encounter difficulties when integrating sustainability with resilience because they were initially conceived to be coherent with the nature of the SC-oriented scope (Pizzol, 2015), but not with the properties of resilience systems. Since resilience can be analysed at different scales, this property has been studied at different levels such as micro (e.g., humans), meso (e.g., organizations), and macro level (e.g., societies) (Bergström & Dekker, 2014). Consequently, studies that adopt an SC-oriented scope (e.g., studies) can reach, at most, a meso level view of resilience since they are focused just on the company or a specific product. However, to the best of our knowledge, even studies that employed CAS-oriented modelling frameworks still rely on LCA-oriented principles to answer question of system sustainability. Thus, relying just on an LCA approach can limit the extent of the resilience scale that can be adopted, which could also forego all the features that CAS-oriented frameworks provide. In this thesis, we aim to explore resilience of s, which corresponds to a macro level. In this sense, we argue that expanding the system modelling scope to an SN level also requires the expansion of the approach of the SAM so it can be underpinned on the principles of a CAS and macro level resilience.

Aspects such as resilience and network dynamism do not reflect direct consequences for society, but provide insights of SN's capacity to achieve well-being goals even after sudden changes. We envision sustainability as the conceptual umbrella that embeds SN complexity. Thus, the sustainability assessment exercise should organically consider these aspects as well as environmental impacts, society development, and economic prosperity. There are aspects that can be directly and indirectly associated with dimensions of well-being in short and long term. For instance, undesired SN states in terms of unemployment and economic losses can be immediately observed after a disruption. Conversely, the effects that network re-adaptation can generate on global temperature cannot be perceived instantly, but they still have important consequences for future societies. In this sense, we propose the following definition:

Definition 3 *a SN is sustainable if it is capable of contributing to the well-being of current and future societies while ensuring its own adequate functioning during its lifetime.*

This vision emanates from the fact the real global SN fairly fits the CAS definition and from the assumption that computational tools (e.g., ABM) can serve as the operational framework to study SN's complexity.

4.2 Principles of a sustainability assessment approach

Considering complexity as the mandatory component and ABM as the core modelling tool, we ground our sustainability vision on four principles described below.

Principle 1 *Sustainability does not focus on an optimal solution, but on delimiting sustainability boundaries*

By accepting that agents are intelligent and autonomous, finding the solution that optimises the SN configuration seems worthless if it requires us to explicitly modify the topology of the network and the operational configuration of every node. Independent agents may act in ways that are unpredictable and can only depend on the environment, other agents' context, or randomness. This means that the system is not deterministic, and we cannot know if an optimal and unique solution exists. In this situation, the 'most' sustainable solution is practically unreachable. Sustainability is a concept that tolerates nuances in terms of how much a system can improve, but is strict in terms of the limits that a system should not surpass. In this sense, it is more coherent to turn the focus on finding the boundaries in which the SN can still be considered as sustainable. Moreover, when we acknowledge the stochastic nature of the CAS, the analysis can be translated in the exercise of determining the probability of remaining (or becoming) sustainable. These *sustainability boundaries* can be established using well-known metrics (e.g., LCA metrics), but can also be delimited appealing to different indicators (e.g., economic and social metrics) that fit the requirements of the practitioner. In this sense, sustainability can be pictured as a region or regions located in a *multidimensional space* so a variety of different solutions can still be considered as sustainable. SN models designed with different parameters can still lead to sustainable outcomes, which implies that no solution is necessarily better than other as long as they remain in a target *sustainable region*. This region can be interpreted as the space where given societal expectations are fulfilled.

Principle 2 *Nodes achievements are irrelevant if they do not lead to system's success.*

Macchion et al., 2020 conducted a qualitative study on 18 firms in the apparel sector and they showed that structural complexity (also referred as static complexity) influences the adoption of sustainability practices at different levels of a SN. In this case, the first tier suppliers experienced difficulties when different sustainability strategies clashed among the focal-firm and the upstream suppliers. This occurs because practices and policies assumes the involvement of all the elements of the system. If we maintain the assumption of firm's leverage over the SN, the new network configuration can indeed lead to a state of sustainability from the firm's point of view. However, implementing this changes over a SC may have effects on the firms outside of the scope of analysis In such way, we ask ourselves if it is reasonable to think that the addition of firms' sustainability states can indeed be equivalent to the sustainability of the network. Under the SC scope, the focus is on understanding the sustainability of a node and its supply chain, ignoring the performance of other nodes associated to the same network (e.g., competitors) (see Figure 4.1a). In contrasts, when analysing the SN, the attention relies on the network's sustainability rather than specific nodes (see Figure 4.1b). Sustainability in an SN should not be evaluated at a micro scale without considering the macro consequences of the decisions. For instance, firms can implement sustainable practices in order to diminish their impacts and increase their profit, but at the same time they can influence the whole sector's footprint and economy (A. Espinosa & Porter, 2011). One reason is that, while components of some dimensions (e.g., environmental and economical) can be conveniently observed from a micro perspective, others (e.g., biodiversity, cultural and social) necessarily require of a macro view to make sense from them.

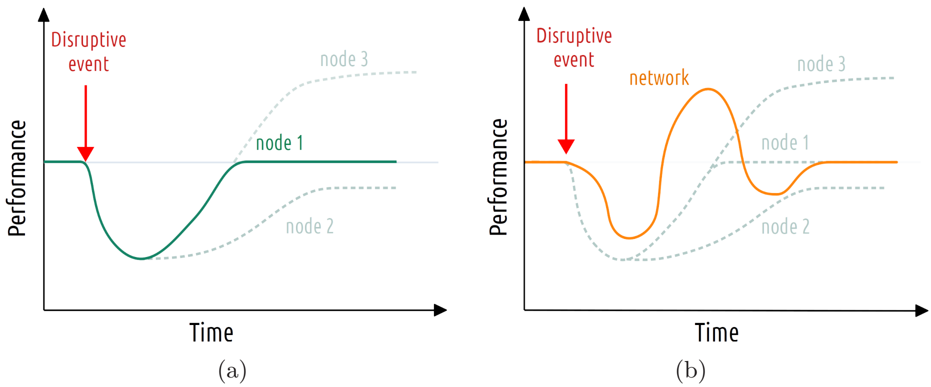


Figure 4.1: Variations on system's performance under a (a) focal-firm oriented supply chain and a (b) non-focal firm oriented supply network

Principle 3 *Shifts the interest from predicting the future towards understanding causalities.*

The SN model is CAS-oriented and the uncertainty of environmental stimuli and agents behaviours may lead to a chaotic system. In this case, attempting to predict a single point in a vast cloud of possible solutions is naive or even erroneous. In an ABM, every action of an agent can be traced back to its behaviour's definition. This means that the sequence of events that occurred during the simulation can be identified and analysed. The coherence among agents' decisions, network topology, and overall indicators must be verified, especially if the programmed rules are meant to be implemented in real life. The agreement between a real-world measurement and the system outcome does not necessarily ensure that the model represents accurately the SN (Oreskes et al., 1994). In this sense, practitioners should not be concentrated on achieving the most accurate prediction because it may deviate the attention from the task of understanding agents' interactions. Because sustainability is now assumed as an emergent behaviour, the key of the assessment exercise is to determine what are the rules or policies that tend to lead to a sustainable system and why is that happening.

Principle 4 *It is dynamic and holistic by nature.*

Society's vision of well-being is not static. Our expectations and tolerances in terms of these *sustainability boundaries* are set on the basis of our appreciation of the current SN state. Hence, due to the network adaptability, some aspects of the state can dramatically change after perturbations as well as the way we value them. After experiencing a highly disturbing event, our main priority may no longer be the minimisation of environmental impacts, but the survival of the economic system and social fabric linked to the SN. This dilemma of objectives, however, should not imply prioritising one over the other, but ensuring the permanence of SN in the *sustainability region*, paying attention to the temporal appropriateness of the considered metrics. For instance, if the network reaches a future state within the expected yearly greenhouse gases (GHG) emissions (i.e., long-term target) without surpassing added value (i.e., short-term target) thresholds during the period of analysis, then we can say this SN is sustainable. In other words, the SN is contributing to the current well-being and ensuring its functioning while being capable of considering the well-being of future societies. On the contrary, if the system is inside this long-term target bounded space, but has highly decreased below any short-term target threshold, we can no longer consider it as sustainable because it cannot ensure its own survival nor its contribution to the economy. For instance, Fig. 4.2 depicts two systems (i.e., $\boldsymbol{a}$ and $\boldsymbol{b}$), evaluated using two sustainability metrics after a disruption occurring at time t_1. System $\boldsymbol{a}$ is considered sustainable because it does not surpass the short-term (added value) and long-term (CO_2eq/year) imposed emission threshold, measured at t_2 and t_4, respectively. In contrasts, system $\boldsymbol{b}$ cannot be considered as sustainable because it surpasses the threshold in t_2, despite having a better performance in t_4 for both yearly emissions and added value indicators.

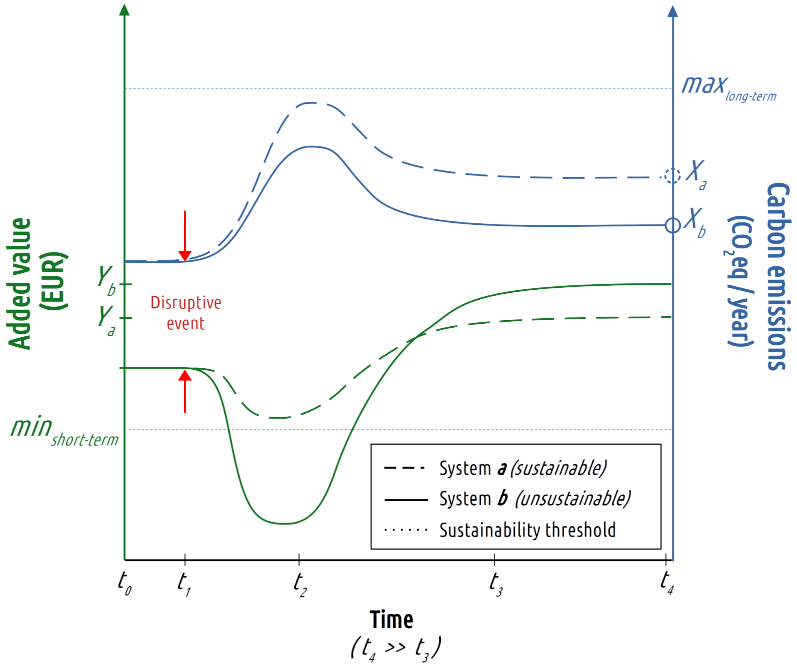


Figure 4.2: Performance of a sustainable (***a***) and an unsustainable (***b***) system under the evaluation of a short-term (added value) and a long-term (carbon emissions) sustainability indicator after a disruptive event.

Under this approach, we do not need to use proxies to describe systems proneness to failure because we can observe explicitly how the network and metrics vary after the introduction of disruptive events. For this, metrics should be carefully selected so they can indicate if the SN is still functioning or has failed. In this sense, a SN can be called robust if it remains inside the *sustainable region* and does not experience dramatic changes during the whole simulation, implying that it has the capacity of coping with external disturbances. Similarly, a SN can be considered as resilient if it can return to a position distant from the *sustainability boundaries* after approaching them. This means that the SN has the capacity of returning to its initial state after being negatively affected by disruptive events. With this logic, a system that surpasses the imposed thresholds cannot be called as unsustainable even if it eventually returns to its initial condition. It is important to notice that the main focus is not on finding a resilient or robust configuration because they are structural aspects embedded into the sustainability analysis process we propose. By embedding the short-term effects, the necessity of determining if a system is resilient or robust becomes overshadowed by the sustainability target.

4.3 Towards a new sustainability assessment framework

The proposed principles represent a conceptual basis that can be used as a compass to design an assessment method. Based on these, we identified a potential path to develop a complexity-driven SAM to be used when analysing disruptions or other complex phenomena in SN (see Fig. 4.3). The following set of stages describe a framework that should allow the modelling of a SN and potential disruptions, nodes' interactions, and should deliver enough information for decision-making. This framework involves sequential steps and heuristics that provide the notions to couple SN topological aspects and sustainability principles in a practical manner during the computational phase and the decision-making exercise.

4.3.1 Computational modelling of the supply network

The modelling stage should consist in representing the industrial sector we aim to evaluate as a network of agents. Ideally, agents should always depict real-world entities, meaning that firms as well as key stakeholders need to be included into the network. Moreover, aspects such as firm's production scheme and emission factors, selling and procurement behaviours, and managers' mitigation plans need to be considered. It is unpractical and sometimes unfeasible to collect detailed data of every firm. Thus, relevant companies need to be identified so they can be explicitly represented, while the remaining can rely on secondary data or experts opinions. Once the elements of the SN have been mapped, agents need to be represented as computational objects with attributes and functions. For this, any ABM tool can be used as long as it allows to program explicit agents' characteristics, account for interactions, consider current sustainability metrics, and treat the SN as a computational graph object. Finally, companies' characteristics will then be ingested as attributes and decision rules as functions.

4.3.2 Selection of parameters and events of interest

Once the computational engine of the simulation is set, the next step should be to identify the different parameters that will vary during each simulation. The logic behind considering more or less parameters responds to expected influence of those over the system behaviour. These influences are usually based on evidence or can be assumed a priori as part of the research hypotheses. Parameters such as production capacity, initial position of an agent in the network, emission factors, delivery time and efficiency tend to determine the performance of a company in the market. We label these as *endogenous parameters* because they are intrinsic to agents and vary according to firms' access to information. On the contrary, we label aspects such as market demand, environmental and anthropogenic disruptions, and public policies as *exogenous parameters* because they are context dependant and do not rely on a particular agent state or point of view (see Fig. 4.3). Both of these parameters are meant to be set before the simulation run as initial conditions.

There may exist parameters from these two categories that are not expected to remain constant because of the uncertainty associated with them. In ABM exercises, it is usual to assign a probability distribution to these parameters to provide a computational source of randomness into the modelling. By this, real-world randomness can be measured and it promotes agents to encounter always different decision situations. In this sense, it is evident that multiple simulation runs with same initial conditions (e.g., Monte Carlo simulation) need to be performed to make sense of the stochastic nature of these parameters. In a similar way, events of interest (e.g., disruptions) are meant to be programmed and included into the model. For instance, natural phenomena can be introduced indirectly as slight variations in some environmental parameters used by agents, such as precipitation (i.e., required by farmers), or change in availability of a natural resource (i.e., fishes at the ocean). Other disruptions, like explosions or lock-downs, can be introduced as direct changes in network's topology, such as the deletion of nodes in a certain country or region or the instant variation in production capacity of certain firms. Moreover, the practitioner has to explicitly program the start and end of the exogenous disruptive events over the simulation environment so it can be executed during run-time. Finally, the combination of all the parameters and events of interest will set the conditions of the simulation which we can label as a *scenario*.

4.3.3 Validation and simulation of scenarios

A priori assumptions and model outcomes have to be verified and validated before using the model in any assessment exercise. For this, a set of indicators or metrics should be proposed, so they can be interpreted as time dependant variables that represent the state of the SN in a given time step. The practitioner's task is to make sense from these metrics and validate or reject the SN topology and outcomes. There are multiple metrics that can be used to characterise the simulation results, but depending on the nature of the indicator, we can classify them into *system metrics* and *target-oriented metrics*. The former represent performance and structural properties of the system that can be used as proxies to describe network's topology, but cannot be explicitly related to a sustainability state. The latter are metrics that can be directly associated with society's vision of well-being and can be used as dimensions of the *multidimensional space*.

On the one hand, network analysis indicators, such as centrality measures and their distributions, can be directly used as *system metrics* and they also serve to validate model's capacity of simulating a feasible SN topology. Moreover, indicators like betweenness or alpha centrality (Borgatti et al., 2009) can be used to identify relevant agents and to track their roles in the SN during the simulation. On the other hand, indicators used in LCA (e.g., global warming potential, water depletion), life-cycle costing (e.g., value added), or social LCA (e.g., direct employment) can be used as *target-oriented metrics*. For this kind of metrics, new indicators can be proposed as long as they can be calculated from the simulated SN and associated with dimensions of sustainability or society goals.

Given the stochastic nature of ABM and the high degree of freedom of the parameters space, the model validation exercise consists on the selection of the vector of parameters that yields results that approximate the most to the selected validation metrics. This can be achieved by exploring the results through iteratively sampling from the parameter space, until the approximation to the metric is considered adequate (Lamperti et al., 2018).

With the computational engine, parameters and metrics configured, the next step will be to run one simulation for each scenario, or multiple simulations if the scenario is bounded with uncertainties that are meant to be evaluated (e.g., Monte Carlo simulation). A simulation run for one scenario will generate a set of $\boldsymbol{t}$ graphs, and a set of $\boldsymbol{t}$ vectors of dimension $\boldsymbol{m}$ containing the network and the values of $\boldsymbol{m}$ *target-oriented metrics*, respectively, for every time step from 0 to $\boldsymbol{t}$ (see block 3 in Figure 4.3). The first set should be used to calculate all the *system metrics* and to understand the changes in the SN topology, while the second set can serve to position the SN state in the *m-dimensional space* conformed by every *target-oriented metric*.

4.3.4 Sustainability space identification

In this stage, *sustainability boundaries* can be introduced as upper or lower thresholds for every *target-oriented metric*. For instance, in a three-dimensional space the thresholds can be graphically represented and the *sustainability region* can be intuitively distinguished (see block 4 in Figure 4.3). In this sense, the sustainability of a SN state is determined by the location of its coordinates in the *multidimensional space*. When the stochastic nature of the parameters is considered by performing a Monte Carlo simulation, for instance, the multiple simulations will lead to a cloud of points. In this case, the interpretation cannot be dichotomous anymore (i.e., it is or not sustainable), but it has to consider the distributions of the simulations for every dimension (i.e., the probability of staying in the sustainable region). It is not practical to perform this graphical analysis of the SN state and the *multidimensional space* $\boldsymbol{t}$ times. Because of this, the ABM should be equipped with tools to automate the process of calculating the distance of a point to the boundaries in an *m-dimensional space*.

4.3.5 Analysis and decision making

This stage should be used to interpret the simulations and to generate knowledge from it. The type of analysis may vary depending on the objective of study. For instance, when designing a SN it is relevant to explore and identify the operational configuration most likely to lead to a sustainable state. If the goal is to explore the effects of disruptions then it will be important to identify the nodes that play crucial roles in sustainable or unsustainable SN states. If the objective is to test new policies, theories or rules, node interactions and cause-effect chains can be examined step-by-step to make sense of the action mechanism that lead to the final state.

The simulations generate a synthetic database that can be also used with data analysis purposes. When many samples of the parameters space are simulated, the results can serve as inputs of a surrogate model or meta-model, so a more extensive analysis can be performed efficiently. A meta-model is a model representing the behaviors of the original model, but with a higher level of abstraction (Pietzsch et al., 2020). In this way, further exploration do not require the simulation of new inputs, but the analysis of input-output relationship identified in the meta-model (Edali & Yücel, 2019). For example, the influence of certain initial parameters in the sustainability state can be studied. Moreover, the metamodel could be used to map initial conditions to the likelihood of remaining in the *sustainable region* can be developed using statistical or machine learning approaches. The objective of this modelling strategy is to avoid the necessity of running simulations if the influence of certain parameters in the model output has been identified and validated.

Finally, this stage does not represent utterly the final phase because it can be in the middle of multiple iterations steps in the process of achieving the right model. Validation, verification and calibration processes may require to traverse all the different steps presented before.

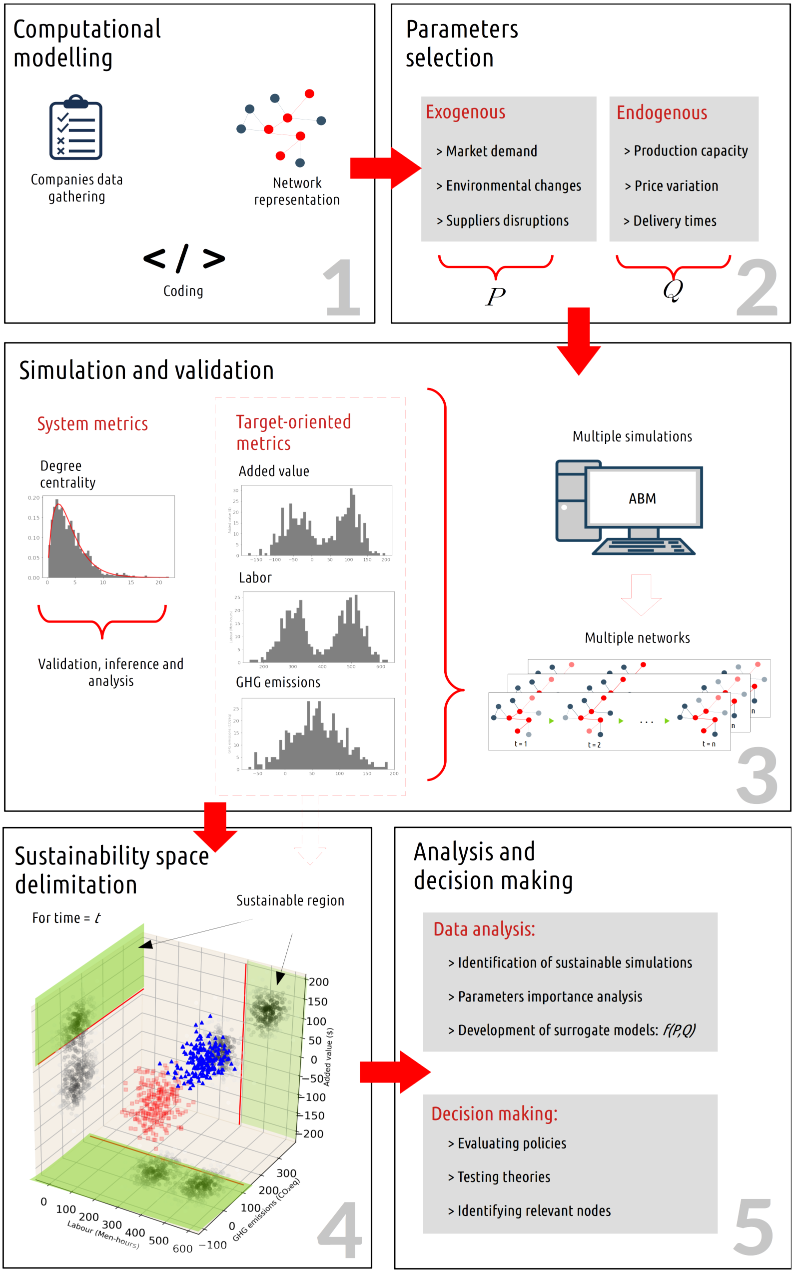


Figure 4.3: Required stages for a potential framework of a complex-oriented sustainability assessment method for supply networks.

Chapter 5

Summary Part I

The conceptual map in Fig. 5.1 summarizes the findings of this part. We conducted a non-systematic literature review in order to understand the methodological barriers in the assessment of complex systems. More specifically, we focused on understanding the characteristics of both resilience and sustainability as part of the same assessment framework. From the literature, we identified three types of decoupling when it respects to including these two concepts in the modelling exercise: methodological, motivational, and temporal decoupling. Moreover, in addition to this decoupling, we found that modelling SNs represents a challenge because of their complexity from an algorithmic, a deterministic, and an aggregated perspective. We leveraged on our findings to propose four principles that should comform a complexity-oriented sustainability assessment approach. Finally, this conceptual development was used to present a sustainability assessment framework that relies on ABM as its core methodology.

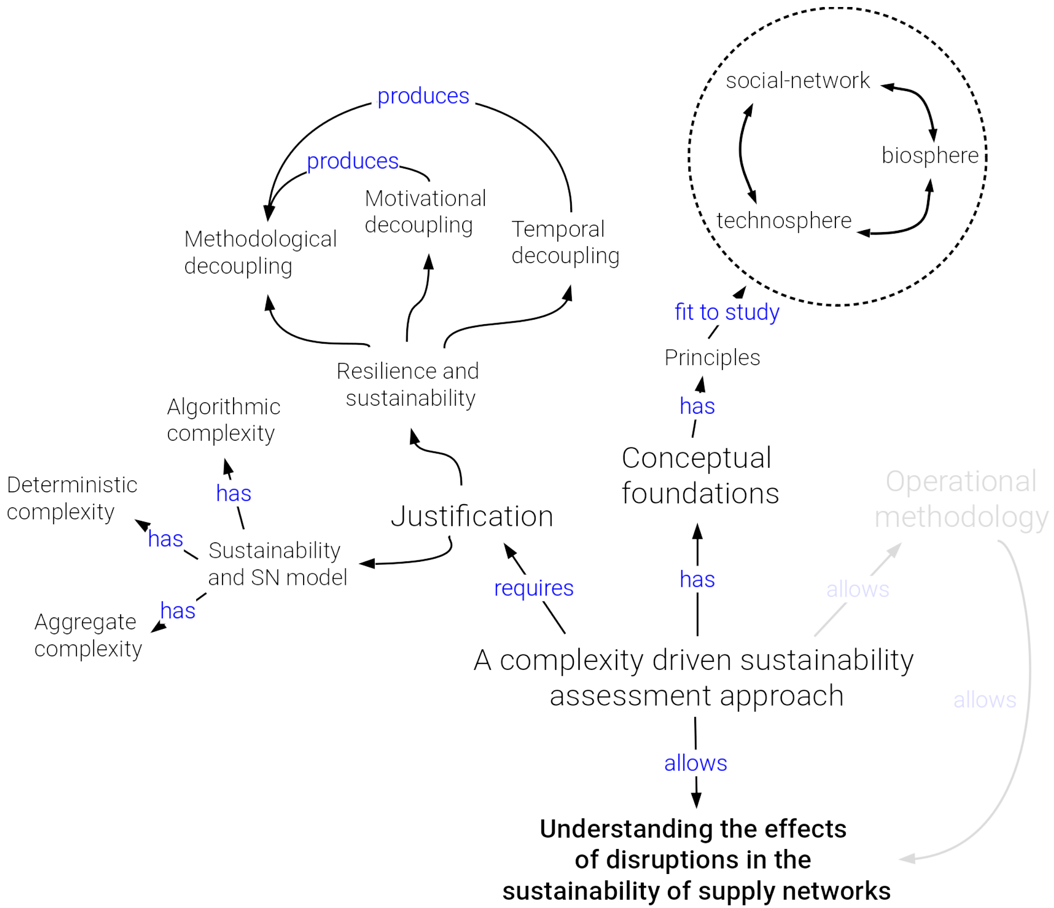


Figure 5.1: Expanded conceptual map of the aspects developed in chapter 4

Part II

An operational framework for modeling socio-technical system

Chapter 6

AFRICA: an Algebraic Framework for RepresentIng Computational Agents in socio-technical systems

List of symbols

P_ω Set of products considered in ω operational configuration.

P Set of all products flowing through the supply network, where $P = \bigcup_{\omega\in\Omega} P_\omega$.

S_ω Set of processes considered in ω operational configuration.

Ω Set of all agents.

$\boldsymbol{A}$ Decision matrix with dimensions $n \times m$ and entries $a_{i,j}$.

$\boldsymbol{F}$ Factor requirements matrix with dimensions $o \times m$ and entries $f_{k,j}$.

$\boldsymbol{Q}$ Impact matrix with dimensions $l \times m$ and entries $q_{b,j}$.

$\boldsymbol{\kappa}$ Cost vector.

$\boldsymbol{\phi(\cdot)}$ Function that solves an instance of the sourcing problem.

$\boldsymbol{\theta}$ Operational configuration.

$\boldsymbol{e}_j$ $j-th$ standard basis vector of $\mathbb{R}^m$.

$\boldsymbol{y}$ Demand vector.

ω A socio-technical agent, where $\omega \in \Omega$.

b Rows indexer for $\boldsymbol{Q}$.

i Rows indexer for $\boldsymbol{A}$, $\boldsymbol{y}$.

j Columns indexer for $\boldsymbol{A}$, $\boldsymbol{F}$, $\boldsymbol{Q}$, $\boldsymbol{s}$.

k Rows indexer for $\boldsymbol{F}$, $\boldsymbol{\kappa}$ or $\boldsymbol{c}$.

m Number of processes contained in a set S_ω, where $m \in \mathbb{Z}$.

n Number of products contained in a set P_ω, where $n \in \mathbb{Z}$.

$z_\$$ Expenditure capacity.

SNs are considered as demand-driven and they respond, directly or indirectly, to the requests of final consumers. SNs are now more complex and intertwined than ever and the need of broadening our understanding of joint consumption and production systems has motivated the adoption of a more complexity oriented vision in the field of Industrial Ecology (Dijkema & Basson, 2009; Dijkema et al., 2015). Recent events have exposed the susceptibility of global logistics, health systems, and social fabric to unexpected disruptions and changes in consumer behaviors (Béné et al., 2021; S. Singh et al., 2020). This susceptibility has reaffirmed the necessity of understanding system's evolution and adaptation capacity as well as the consequences that this dynamism may have on achieving the sustainable development goals, one of the most important and urgent challenges for current society (Larrea-Gallegos et al., 2022; Sachs, 2012). These targets are ambitious and the progress in making changes in this direction has been held back due to high degrees of inertia exhibited by production and consumption systems (Lebel & Lorek, 2008; Markard et al., 2020; Sachs et al., 2019). In this sense, it is necessary to have the capacity of proposing effective policies considering consequences at both production and consumption levels (e.g., standards, incentives, subsidies and taxes), and to analyse them in terms of the feasibility of their implementation and the actual reduction of the evaluated impacts. This implies that the SN modelling exercise requires to be capable of including aspects of complexity and human behavior, as well as the bidirectional influence of consumption side over the SN.

6.1 Introduction

Incorporating human behaviors into the design of a technical system is not trivial because social and technical systems can be modeled using different assumptions, structures, and problem-solving strategies (Bettencourt & Brelsford, 2015). As shown in chapter 2, migrating from a technical to a STS approach cannot be achieved effortless since different layers of difficulty arise, such as the introduction of structural properties into the sustainability assessment, or the novel exercise of modelling producers and consumers in the same computational framework. This challenge was previously discussed in the literature, where it has been noted that current analytical assessment frameworks, such as LCA, are limited when it refers to studying these properties in full detail (Meerow & Newell, 2015; Pizzol, 2015). In fact, to the best of our knowledge, only the Stochastic Technology-of-Choice Model (STCM) has been able to incorporate aspects of decision-making in an analytical manner by integrating aspects of linear programming and algebraic LCA along with factors and constrains (Katelh ön et al., 2016).

As found in literature reviews (Baustert & Benetto, 2017; Micolier et al., 2019), most of ABM implementations are done by adopting partially or entirely the LCA analytical framework. This has been predominantly done to evaluate the adoption of sustainable attitudes towards procuring and technology selection (C.

Davis et al., 2009; Lan & Yao, 2019; Navarrete Gutiérrez et al., 2015) or modelling changes in the use phase of a product (Grant & Hicks, 2020; Raihanian Mashhadi & Behdad, 2018; Walzberg et al., 2019). All the studies found in literature rely on different ontology, operational frameworks and simulation environments, which makes the models case-specific. We identified that only C. Davis et al., 2009 provided a formalisation and ontology general enough to be considered as a replicable framework. C. Davis et al., 2009 introduced general concepts like *operational inputs and outputs* and *operational configuration* that have been implicitly utilised in posterior ABM implementations. Despite this, developing the ABM was not trivial since practitioners required to implement a simulation environment that allowed agents to interact independently and representing agents' technical characteristics and behavioral mechanisms as computational objects.

We prioritise our effort on developing a solution to overcome the difficulty of representing agents as computational entities. Namely, company's technological and social aspects require to be represented in code following a computational framework that needs to be compatible with the behaviors or decision mechanisms considered in the modelling (e.g., technology selection, supplier selection, behavior diffusion, etc). Depending on the considered mechanisms, the complexity of the implementation can range from simple predicates (e.g., if-then statements) to more elaborated computational structures. Moreover, since different code can still yield to the same functionality, practitioners tend to adopt different strategies when programming without relying on any formal computational framework (Baustert & Benetto, 2017; Micolier et al., 2019). In practice, literature shows that the logic and structure for representing computational agents can differ greatly from model to model despite dealing with the same type of socio-technical agents (i.e., producers and consumers with inputs and outputs). This lack of consistency yields the development of large models with ad-hoc designs (An et al., 2021). Meaning that practitioners repeat the effort of designing computational structures and implementing them in code with every new case of study (e.g., new research question, different industry, or new behavioral mechanism). Moreover, the variety of programming languages and simulation environments (Abar et al., 2017) makes current ABM models language-dependant and case-specific, limiting the capacity of recreating and validating results, or building on top of ongoing research. We argue that the required additional effort, and the lack of flexibility and replicability can limit the usefulness of ABM as a tool for solving sustainability-related inquires, and consequently, discourage the use of this paradigm when dealing with complexity-related questions that can contribute to achieve sustainability development goals.

6.2 A novel framework proposal

We focus our attention on the absence of a common framework for modelling production and consumption entities, for which we propose an Algebraic

Framework for RepresentIng Computational Agents (AFRICA). AFRICA is a comprehensible, reusable, and flexible mathematical framework for programming socio-technical agents in ABM. The motivation behind proposing AFRICA is to have a basic and reusable structure to describe agents' technological system while still allowing the introduction of non-technical constrains in a systematic manner. In this sense, the utility of AFRICA relies on four main characteristics. Firstly, the elements depicted by the framework manage all the numeric information that describe agent's operational configuration as mathematical objects (i.e., arrays) in the form of matrices and vectors. Secondly, it is flexible enough to represent technical or socio-technical aspects of most types of SN entities (e.g., resource extractors, producers, traders and consumers) without altering the basic components and properties initially defined by the framework. Moreover, it can be used when studying different action mechanisms and behaviors from both production and consumption side (e.g., sourcing problem, production planning, consumption problem). Thirdly, it is language-agnostic because its mathematical structure allows to implement it in any ABM in a comprehensive and reusable way regardless of the selected programming language or the architecture of the simulation environment. Finally, it is built on top of state of the art, which results from rethinking and adapting sustainability assessment notions (i.e., LCA and STCM) (Heijungs & Suh, 2002; Katelh ön et al., 2016), making it coherent and compatible with others computational resources like environmental databases (i.e., ecoinvent 3).

In this sense, we argue that our framework provides an useful and robust alternative for representing producers and consumers simultaneously when building ABM models in sustainability assessment. Indeed, by facilitating the adoption of a STS approach, practitioner's inquiries can range from conventional sustainability assessment tasks (e.g., product's impact) to complex behavioral-related questions (e.g., environmental consequences of consumers response to a policy) using the same modelling paradigm. We also demonstrate this statement by providing a proof of concept in which we explore fundamental notions and effects of the introduction of sustainable behaviors in a production-consumption network (see Part III, section 9). For this purpose, we formalize the framework, its mathematical elements and their properties in section 6.3. Then, the features of AFRICA are visually explained in section 6.4). Finally, section 6.5 presents a numeric example in which the expected used of the framework is shown.

6.3 AFRICA algebraic framework

Our framework is strongly underpinned by the mathematical elements used in the STCM (see Section A for a comprehensive description of STCM). However, differently from the STCM model, we do not assume that the entire chain of processes responds to common and unique objective (e.g., cheapest production pathway). On the contrary, AFRICA is designed to operate under the assumption that the SN is a CAS and that its final state emerges from the interaction and adaptation of rational agents. In this sense, system's flows can only be determined after solving each individual socio-technical decision problems. In ABM, rational agents are commonly modeled following the belief, desire and intention concepts in a so-called belief-desire-intention (BDI) architecture, which allows modellers and end-users to handle agents in comprehensive and easier manner (Adam & Gaudou, 2016; D. Singh et al., 2016). In this section, we follow a similar fashion where *beliefs* represent agent's knowledge about the world, *desires* indicate objectives, and *intentions* are the actions that will lead to achieving agent's objectives.

We consider the sourcing decision problem -sourcing problem hereafter- to exemplify a conventional decision dilemma every socio-technical agent $\omega \in \Omega$ needs to solve. The sourcing problem consists in determining the adequate combination of transformation processes, suppliers (e.g., cheaper or greener supplier) and supplies (e.g, ideal technologies and optimal amounts) that allows the generation of an output product. This is the initial step of any procurement process, and it provides key information for other decision steps (e.g., production, purchasing, quotation, etc). Agents are meant to solve an instance of a sourcing problem every time they aim to satisfy a demand, whether it is real or expected. This demand can be imposed by other producer agents (e.g., companies purchasing or requesting quotation), consumers (e.g., households or end users), or self-imposed (e.g., agent deciding to stock up). For instance, in a simple SN and for a given producer agent ω_1, the sourcing problem will consist on deciding the combination of inputs that will let it satisfy a demand $\boldsymbol{y}$ (see Fig 6.1b). This decision does not only involve ω_1's technologies, but also the possible business interactions with other agents and their available technologies (see Fig 6.1a). In this sense, we depict the system as a composition of social agents strictly constrained by technological components.

6.3.1 Actions boundary and decision space: formal definitions

A set P_ω includes all the n products that are consumed or produced by agent ω. Thus, the union of every agent's products yields the set P, which contains all the products flowing through the SN. In a similar way, we can define a set S_ω which contains all the processes that consume or generate the products in P_ω. While products in P_ω may be common among agents (e.g., diesel as an input) (see Fig 6.1a), elements in a set of processes S_ω are exclusive to each agent ω since they describe its own variety of possible alternatives for sourcing goods. We label the space created by all the available processes of ω as the its *decision space*. This space has a dimension $m = |S_\omega|$ and it is defined by all the possible combinations in terms of quantities and processes to be decided on (i.e., $\mathbb{R}^m_{\geq 0}$). In the previous example of ω_1, the *decision space* can be illustrated as a network of available processes and products shown in Fig. 6.1c.

Based on the degree of agent's influence over different possible processes, we classify these in three types: production processes, storage selection processes, and purchasing processes. Production processes describe transformation activities directly performed by the agent ω or under its direct responsibility. Storage selection processes are activities that represent the action of retrieving finished goods from one or multiple storage facilities controlled by agent ω. Finally, purchasing processes describe the activity of buying products from other supplier agents or markets through potential transaction activities. In this case, purchasing to a market denotes the acquisition of products from an average and unconstrained supplier. Markets are entities that lack of agency and they can be interpreted as proxy-agents that represent a share of an industry not covered by agents in $\Omega \backslash \{\omega\}$, guaranteeing successful computation even in the absence of supplier agents.

Decisions of agent ω regarding purchasing processes only reflect the intention of acquiring an amount of product from another agent, but not the proper action of purchasing the product itself. The agent believes that the purchasing action can be performed because it assumes that all processes in the *decision space* are feasible and based on beliefs that match reality. However, supplier agents could reject the purchase request for multiple reasons (e.g., particular strategy, false information, etc), meaning that ω has no means to guarantee a successful purchase. In this sense, we define the *actions boundary* as a delimitation that encompasses only the processes that are under complete control of ω, such as production and storage selection processes. In the *decision space* illustrated in Fig. 6.1c, the green colored processes belong to ω_1's *actions boundary*, while the blue and gray correspond to purchase processes that are bounded to other agents' state.

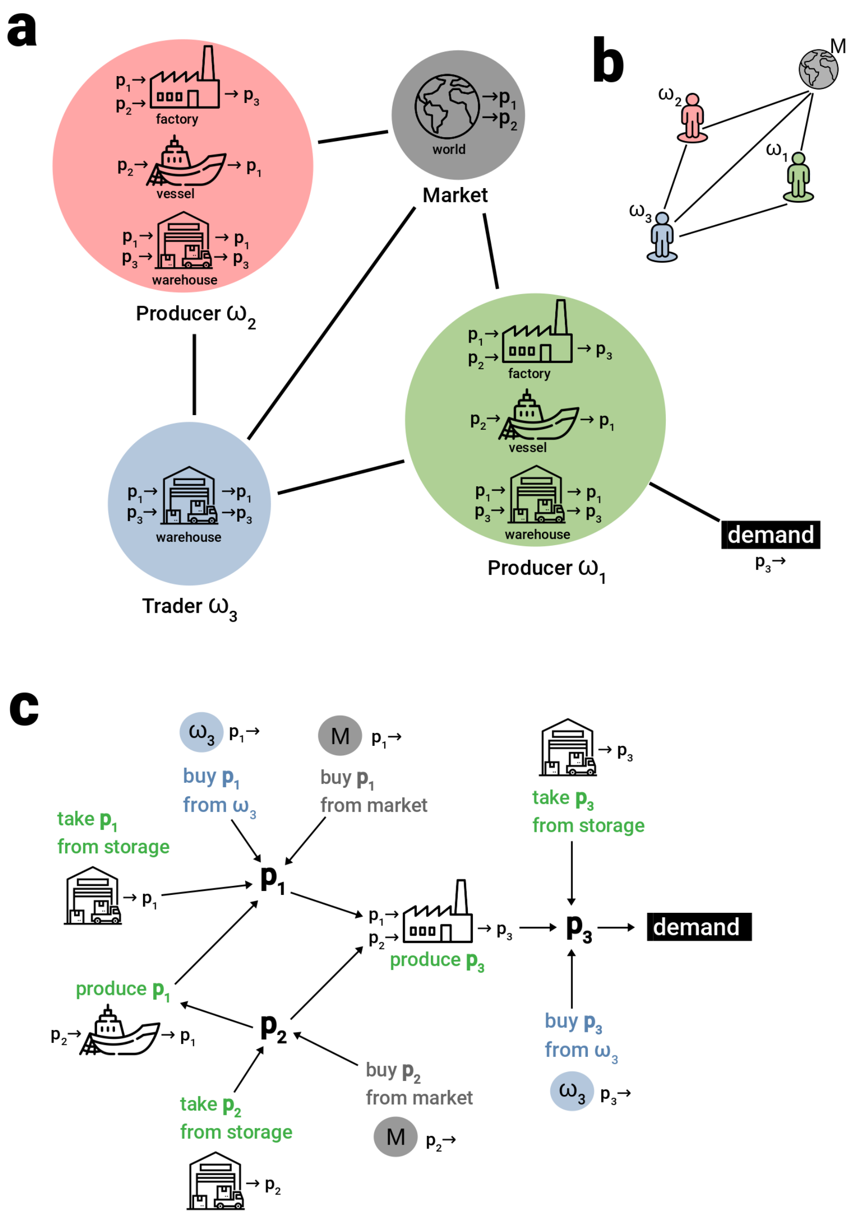


Figure 6.1: Example of a supply network composed by $\boldsymbol{\Omega} = \{\omega_1, \omega_2, \omega_3, M\}$ with $\boldsymbol{P} = \{p_1, p_2, p_3\}$ products and an imposed demand for product p_3 (a). The network is depicted as a system of social agents (b) constrained by technical components. (c) shows the *decision space* of a producer agent ω_1 that aims to satisfy a demand of product p_3. Processes in the *actions boundary* are colored green, while blue and gray colored processes refer to interactions with other agents

6.3.2 Agent's *operational configuration*

To describe agents characteristics, we leverage on the definition of *operational configuration* which was proposed by C. Davis et al., 2009; Nikolic and Ghorbani, 2011 to hold information about products' inputs and outputs as part of their computational agent's ontology. Similarly, in AFRICA, an agent's *operational configuration* consists on the elements (i.e., vectors and matrices) containing enough information to formulate and solve an instance of the sourcing problem, or any other more sophisticated business decision problem (e.g., inventory selection, principal-agent problem or logistics). These elements represent the relationship among processes, products and factors, where products are produced or consumed by processes, and processes are constrained by factors (Katelh ön et al., 2016). The elements of the *operational configuration* will be constantly called during every time step t of a simulation of T days, meaning that they are meant to be instantiated for every agent before run-time. Moreover, the structure of the *operational configuration* is such that it allows to represent the concepts of *decision space* and *actions boundary* in a structured manner. Every agent ω has an *operational configuration* described by three matrices (i.e., decision, factor requirements and impacts), four vectors (i.e., constrains, total cost, demand, and supply) and one scalar (i.e., expenditure capacity). All elements in the *operational configuration* are dynamic, meaning that they can be updated at every time step t whenever new information is acquired. These components are formally introduced as follows:

Decision matrix The decision matrix $\boldsymbol{A}_{n\times m}$ describes the relationships between products and processes present in the *decision space*. Every entry $a_{i,j}$ associates a product i with a process j that consumes it or generates it, whether the process is under agent's control (i.e., production and storage selection), or bounded to another agents' state and objectives (i.e., purchase). When $a_{i,j}$ has a positive sign, it indicates that product i is an output of process j, while a negative sign indicates that it is an input. A process j can deliver multiple products (i.e., co-products), but the magnitude of values should be such that they are proportional to an unit of one of the outputs. In other words, when process j has a reference product i, values in column $\boldsymbol{A}_{:,j}$ should be interpreted as "*the products required by process j to deliver one unit of product i*". By this way, reference products can be identified wherever $a_{i,j} = 1$. Every product i must be a reference product in at least one column, whether it corresponds to a production, storage selection, or purchasing process (i.e., $\forall i \in \{1, \ldots, n\}, \exists a_{i,j} = 1$). This means that, at minimum, matrix $\mathbf{A}$ will be square, which implies that $m \geq n$ for all cases. The selection of a reference product among outputs could be arbitrary, but it is recommended to follow a logic where the reference product is the one that determines the production while the rest of outputs depend on it (Weidema et al., 2018).

Factor requirements matrix Matrix $\boldsymbol{F}_{o\times m}$ describes physical and non-physical factors[1] that are requirements of processes in the *decision space*. Each entry $f_{k,j}$ describes the amount of factor k required by process j to deliver one unit of its reference product. Factors represent criteria that may affect decision making during production (e.g., labour, operation of machinery), storing (e.g., storage capacity, transportation effort) and acquisition activities (e.g., delivery time, purchasing action).

Total, embodied, and direct impact matrices The total impact matrix $\boldsymbol{Q}_{l\times m}$ describes the impacts associated with *decision space*. Every entry$q_{b,j}$ represents the amount of social or environmental impact b associated with a unitary output of process j. This matrix depicts, implicitly, the cause-effect relationship between the *decision space*, and the space conformed by natural resources, the environment and human society. $\boldsymbol{Q}$ is the aggregation of an embodied and a direct component, being the former the impact previously generated, and the latter the impact that will occur immediately after the decision is taken. For instance, for a *storage selection* process the embodied component will be the life cycle impact of the product stored in the facility, while the direct component is zero since no impact is generated from choosing a product already manufactured. Analogously, for a *production* process, the direct component corresponds to the impacts of transforming the inputs (e.g., combustion emissions), while the embodied component is zero since the process is only referring to an instantaneous transformation of materials. In this sense, matrix $\boldsymbol{Q}$ can be expressed as the sum of an embodied impact matrix$\boldsymbol{Q}^e$ and a future impact matrix $\boldsymbol{Q}^f$. A decision where impacts follow a life cycle perspective should use the matrix $\boldsymbol{Q}$, while a decision considering only direct impacts[2] should use matrix $\boldsymbol{Q}^f$.

Total, embodied and future cost vectors Total cost vector $\boldsymbol{\kappa}$, of size o, provides a notion of the monetary cost[3] of using one unit of factor k present in matrix $\boldsymbol{F}$, where a value of zero can be assumed when monetising is not possible or to indicate a free factor. This vector represents an aggregation of agent ω's beliefs regarding the cost of consuming one unit of factor k and beliefs regarding any embodied cost or expense previously associated to that factor. In this sense, $\boldsymbol{\kappa}$ is the sum of an embodied cost vector $\boldsymbol{\kappa}^e$, and a future cost vector $\boldsymbol{\kappa}^f$. For example, a *storage selection* process has an embodied cost equal to the cost already paid when acquiring the stored good, while its future cost is zero since there are no additional costs involved in selecting the good. In the same manner, a *production* process has a future cost that represents the

[1] Differently from Katelh ön et al., 2016, we contemplate the possibility of using non-physical factors as long as prices and constrains units are consistent

[2] In the computational structure of LCA (Heijungs & Suh, 2006), matrix $\boldsymbol{Q}$ does not refer to impacts but the characterization factors. In AFRICA we refer directly to the impacts, and we introduce the 'embodied' and 'direct' distinction since temporality is introduced.

[3] Although we link factors with their monetary cost, this can be generalised to consider any "relationship of value". For instance, Larrea-Gallegos et al., 2017 re-adapted this notion to link factors with a "profit vector" in a consequential LCA model

transformation of inputs, while it has no embodied cost since the process only involves a transformation just about to occur. In production, agents willing to exhaust available stocks first should use only $\boldsymbol{\kappa}^f$ (e.g., first-in, first-out strategy) (Morse and Richardson, 1983), while when setting product's price, agents should use $\boldsymbol{\kappa}$ to consider all the expenses.

Constrains vector The constrains vector $\boldsymbol{c}$, of size o, represents the availability each factor k present in matrix $\boldsymbol{F}$. It is based on current agent ω's beliefs, meaning that values in $\boldsymbol{c}_k$ do not necessarily match reality (e.g., inaccurate available stock provided by an unreliable supplier). When the factor k is unconstrained, $\boldsymbol{c}_k$ can be set as ∞.

Demand and supply vectors, and expenditure capacity The demand vector $\boldsymbol{y} \in \mathbb{R}^n_{\geq 0}$ and supply vector $\boldsymbol{s} \in \mathbb{R}^m_{\geq 0}$ can be understood as the question and the answer of the sourcing problem, respectively. The vector $\boldsymbol{y}$ depicts the demand that agent ω is meant to satisfy, while the vector $\boldsymbol{s}$ represents the selected supplies for this purpose (i.e., a quantity from each process). Finally, the expenditure capacity $\boldsymbol{z}_{\$}$ is a scalar that indicates agent's available money.

6.3.3 Construction of the operational configuration

Decision matrix We propose the construction of the decision matrix $\boldsymbol{A}$ in a sequential manner so columns can be indexed in three blocks based on the process types previously described (i.e., production, storage selection and purchasing processes). The first block $\boldsymbol{A}_{prod}$ is composed by columns that describe transformation processes that are under complete control of the agent (i.e., $\boldsymbol{A}_{:,j}, \forall j \in \{1, \ldots, n'\}$). The second block $\boldsymbol{A}_{stor}$ is composed by $n'' - n'$ columns that denote storage selection processes, being n'' the index of the last storage selection process (i.e., $\boldsymbol{A}_{:,j},\ j \in \{n'+1, \ldots, n''\}$). In principle, every product must be associated with at least one storage selection process since products either go to or come from a storage facility. Thus, the minimum amount of storage selection processes is constrained by the amount of products (i.e., $n'' - n' \geq n$), while the maximum corresponds to all the possible combinations between n and available storage facilities. The third block $\boldsymbol{A}_{supp}$ has $m - n''$ columns, and it contains the remaining processes that represent the intention of purchasing a product from another agent or market (i.e., $\boldsymbol{A}_{:,j}, j \in \{n'+1, \ldots, m\}$). For this case, we contemplate the possibility of $m - n' \geq 0$ since an agent could also be a peripheral nodes that lacks of suppliers (e.g., resource extractors). Matrix $\boldsymbol{A}$ is then an augmented matrix that results from appending these three blocks from left to right (i.e., $\boldsymbol{A} = (\boldsymbol{A}_{prod} \mid \boldsymbol{A}_{stor} \mid \boldsymbol{A}_{supp})$).

Factor requirements and impact matrices Since matrices $\boldsymbol{F}$ and $\boldsymbol{Q}$ refer to the same *decision space*, they should be built following the same logic, as show in Fig. (6.2). In this sense, $\boldsymbol{F} = (\boldsymbol{F}_{prod} \mid \boldsymbol{F}_{stor} \mid \boldsymbol{F}_{supp})$ and

$\boldsymbol{Q} = (\boldsymbol{Q}_{prod} \mid \boldsymbol{Q}_{stor} \mid \boldsymbol{Q}_{supp})$. Finally, vectors $\boldsymbol{\kappa}$ and $\boldsymbol{c}$ should be indexed to match the factors depicted in $\boldsymbol{F}$.

$$
\begin{array}{rc}
 & \begin{array}{ccc} \overbrace{\qquad\qquad\qquad\qquad}^{\text{production}} & \overbrace{\qquad\qquad\qquad\qquad}^{\text{storage selection}} & \overbrace{\qquad\qquad\qquad\qquad}^{\text{purchasing}} \end{array} \\
\boldsymbol{A}_{n\times m} = & \left[\begin{array}{ccc:ccc:ccc}
a_{1,1} & \cdots & a_{1,n'} & a_{1,n'+1} & \cdots & a_{1,n''} & a_{1,n''+1} & \cdots & a_{1,m} \\
\vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
a_{n,1} & \cdots & a_{n,n'} & a_{n,n'+1} & \cdots & a_{n,n''} & a_{n,n''+1} & \cdots & a_{n,m}
\end{array}\right]
\end{array}
\qquad
\left.\boldsymbol{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}\right\}\text{products}
$$

$$
\boldsymbol{F}_{o\times m} = \left[\begin{array}{ccc:ccc:ccc}
f_{1,1} & \cdots & f_{1,n'} & f_{1,n'+1} & \cdots & f_{1,n''} & f_{1,n''+1} & \cdots & f_{1,m} \\
\vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
f_{o,1} & \cdots & f_{o,n'} & f_{o,n'+1} & \cdots & f_{o,n''} & f_{o,n''+1} & \cdots & f_{o,m}
\end{array}\right]
\qquad
\left.\boldsymbol{\kappa} = \begin{bmatrix} \kappa_1 \\ \vdots \\ \kappa_o \end{bmatrix} \quad \boldsymbol{c} = \begin{bmatrix} c_1 \\ \vdots \\ c_o \end{bmatrix}\right\}\text{factors}
$$

$$
\boldsymbol{Q}_{l\times m} = \left[\begin{array}{ccc:ccc:ccc}
q_{1,1} & \cdots & q_{1,n'} & q_{1,n'+1} & \cdots & q_{1,n''} & q_{1,n''+1} & \cdots & q_{1,m} \\
\vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
q_{l,1} & \cdots & q_{l,n'} & q_{l,n'+1} & \cdots & q_{l,n''} & q_{l,n''+1} & \cdots & q_{l,m}
\end{array}\right]\Bigg\}\text{impacts}
$$

Figure 6.2: General structural of an agentω's *operational configuration*. Dashed lines separate sub-matrices corresponding to each process type

6.3.4 Solving the sourcing problem

From agent ω's perspective, solving the sourcing problem means determining the most convenient combination of processes and amounts to deliver a certain quantity of output products. An agent determines the convenience of a decision on the basis of their desires (i.e., objectives), relying on their beliefs about itself (e.g., current financial status) and the environment (e.g., available suppliers). The delivery action is mathematically equivalent to mapping $\mathbf{s}$ to a demand vector $\mathbf{y}$, described in (6.1). Since vector $\mathbf{y}$ is always imposed as a request, the modelling exercise will consist on determining how agents will calculate vector $\mathbf{s}$.

$$\boldsymbol{A}\boldsymbol{s} = \boldsymbol{y} \tag{6.1}$$

When $\mathbf{A}$ is square and invertible, there is a unique vector $\boldsymbol{s}$ that satisfies eq. (6.1) for a demand $\boldsymbol{y}$ (i.e., $\boldsymbol{s} = \boldsymbol{y}\boldsymbol{A}^{-1}$). However, since the *operational configuration* is dynamic and agents are expected to interact among each other, new suppliers can be discovered or abandoned. This implies that when $m > n$, eq. (6.1) is undetermined and there may exist infinite solutions for $\boldsymbol{s}$. In this sense, an agent ω should have a particular analytical or heuristic function ϕ, implemented in code, that allows it to determine a valid solution.

We generalise the sourcing problem by considering the existence of a function ϕ parameterised by $\boldsymbol{\theta} = \{\boldsymbol{A}, \boldsymbol{F}, \boldsymbol{Q}, \boldsymbol{\kappa}, \boldsymbol{c}, \boldsymbol{z}_{\$}\}$, that maps $\boldsymbol{y}$ to $\boldsymbol{s}$ (see eq. 6.2). The parameter $\boldsymbol{\theta}$ corresponds to agent's state, represented in this case by its *operational configuration*

$$\phi(\boldsymbol{y}; \boldsymbol{\theta}) = \boldsymbol{s} \tag{6.2}$$

The function ϕ can describe any operation or methodology that solves an undetermined system of equations. However, we focus our attention on mathematical optimisation as the core solving method for two main reasons. Firstly, this method is flexible enough to embed agent's objectives in its formulation and it can be implemented in a straightforward way using the mathematical structure proposed in section 6.3.2. Secondly, mathematical optimisation problems have been widely used as part of the heuristics when dealing with multiple constrains in the sourcing problem (Ding et al., 2005). An optimisation problem can be formulated following different approaches, nevertheless, in this article we present two approaches: monetary optimisation and environmental optimisation.

Monetary optimisation This optimisation approach uses the same principles considered in the works of Duchin and Levine, 2011; Katelh ön et al., 2016; Larrea-Gallegos et al., 2018, but with a focus on individual agents rather than the system technosphere. We assume that the agent will aim for optimal decisions to fulfil its objectives (i.e., to generate revenue) while considering some constraints (e.g., factors). In this manner, we define an optimal supply vector $\boldsymbol{s}^*$ that allows to satisfy demand $\boldsymbol{y}$ while maximising the economic benefit without exceeding $\boldsymbol{z}_\$$. This optimisation exercise consists in constraining the solution space by introducing a set of eq. (6.5) - (6.9) in a linear program that optimises a monetary objective function $\boldsymbol{Z}_\$$. This objective function, shown in (6.3), corresponds to the cost of all consumed factors linked to vector $\boldsymbol{s}$. Since it is plausible that demand may exceed agent's production capacities, we introduce a vector of artificial variables, $\boldsymbol{x}$, to allow feasible solutions even when $\boldsymbol{y}$ cannot be satisfied (i.e., big M method) (Bazaraa et al., 2011). $\boldsymbol{x}$ has size n and $\boldsymbol{x}_i$ indicates the missing quantity to satisfy $\boldsymbol{y}_i$, being it zero when the demand is fully satisfied and greater than zero otherwise. the constant value M in (6.3) is a very big scalar (i.e., relative to the other coefficients) so decision variables $\boldsymbol{s}$ are always preferred over $\boldsymbol{x}$ when minimising. The total cost of the decision (i.e., $\boldsymbol{\kappa}^T\boldsymbol{F}\boldsymbol{s}$) should not exceed the agent's current expenditure capacity, $\boldsymbol{z}_\$$. Due to this, eq. 6.4 ensures that the agent has enough money to pay for the decision. The target demand is imposed in equality (6.5), for which we define $\boldsymbol{y}_{bool} \in \{0,1\}^n$ as the Boolean of vector $\boldsymbol{y}$, which has entries equal to 1 for products with non-zero demand, and zero otherwise. Usage of factors and its maximum availability is depicted in (6.6). Equation (6.7) ensures that $\boldsymbol{x}_i$ is non-zero only when a demanded product $\boldsymbol{y}_i$ cannot be supplied from any production, storage selection, or purchase process. Finally, eq. (6.8) and (6.9) indicate that variables cannot be negative.

$$
\begin{aligned}
\min \qquad & \boldsymbol{Z}_\$ = \boldsymbol{\kappa}^T\boldsymbol{F}\boldsymbol{s} + M\boldsymbol{x} && (6.3)\\
\text{s. t.} \qquad & \boldsymbol{\kappa}^T\boldsymbol{F}\boldsymbol{s} \leq \boldsymbol{z}_\$ && (6.4)\\
& \boldsymbol{A}\boldsymbol{s} + \boldsymbol{y}_{bool}^T\boldsymbol{x} = \boldsymbol{y} && (6.5)\\
& \boldsymbol{F}\boldsymbol{s} \leq \boldsymbol{c} && (6.6)\\
& \boldsymbol{A}\boldsymbol{s} \geq 0 && (6.7)\\
& \boldsymbol{x} \geq 0 && (6.8)\\
& \boldsymbol{s} \geq 0 && (6.9)
\end{aligned}
$$

Environmental optimisation In this approach, it is assumed that agents look towards maximising the environmental benefit of the decision regardless of the involved cost. For this, a new objective function $\boldsymbol{Z}_{env}$, in (6.10), is proposed and it aims to minimise the impact of delivering $\boldsymbol{y}$. This approach optimises $\boldsymbol{s}$ for a specific environmental impact $b \in \{1,\ldots,l\}$ that is prioritised by the agent (e.g, Global Warming Potential). In (6.10), $\boldsymbol{Q}_{b,:}$ depicts a row vector corresponding to the specific impact b. The proposed linear program is then subject to the same constraints, and also requires decision and artificial variables as presented in the monetary optimisation approach.

$$
\min \qquad \boldsymbol{Z}_{env} = \boldsymbol{Q}_{b,:}\boldsymbol{s} + M\boldsymbol{x} \qquad (6.10)
$$

$$\text{s. t.} \qquad (6.4), (6.5), (6.6), (6.7), (6.8), (6.9)$$

6.3.5 Properties

Impact and cost of a decision If we assume that the function ϕ is an implementation of any of the optimisation approaches previously presented, vector $\boldsymbol{s}$ can be obtained by using (6.2). The resulting vector $\boldsymbol{s}$ can be plugged in function μ and σ to get the costs and impacts associated to the decision, respectively (i.e. eq. (6.11) and (6.12), respectively). These functions are parameterized by columns indexes j and d, allowing the calculation of the impact and cost for each process type. $\boldsymbol{e}_j$ denotes the j-th standard basis vector of $\mathbb{R}^m$, and $(\sum_j^d \boldsymbol{e}_j \boldsymbol{e}_j^T)$ is a square zero matrix of size m where only the diagonal elements from j to d are 1. This diagonal matrix allows to keep a specific range of values in vector $\boldsymbol{s}$ while assigning zero to the rest. In this sense, costs from production μ_{prod}, storage selection μ_{stor}, and supplier processes μ_{supp} can be calculated using eq. (6.13), (6.14) and (6.15), respectively. In an analogous way, impacts σ_{prod}, σ_{stor} and σ_{supp} can be calculated using eq. (6.16), (6.17) and (6.18), respectively. The total cost μ_{tot} and total impact σ_{tot} can then be calculated using eq. (6.19) and (6.20).

$$\boldsymbol{\kappa}^T \boldsymbol{F} (\sum_j^d \boldsymbol{e}_j \boldsymbol{e}_j^T) \boldsymbol{s} = \mu(j, d) \tag{6.11}$$

$$\boldsymbol{Q} (\sum_j^d \boldsymbol{e}_j \boldsymbol{e}_j^T) \boldsymbol{s} = \sigma(j, d) \tag{6.12}$$

$$\mu(1, n) = \mu_{prod} \tag{6.13}$$

$$\mu(n+1, n\prime) = \mu_{stor} \tag{6.14}$$

$$\mu(n\prime+1, m) = \mu_{supp} \tag{6.15}$$

$$\sigma(1, n) = \sigma_{prod} \tag{6.16}$$

$$\sigma(n+1, n') = \sigma_{stor} \tag{6.17}$$

$$\sigma(n'+1, m) = \sigma_{supp} \tag{6.18}$$

$$\mu_{prod} + \mu_{stor} + \mu_{supp} = \mu_{tot} \tag{6.19}$$

$$\sigma_{prod} + \sigma_{stor} + \sigma_{supp} = \sigma_{tot} \tag{6.20}$$

Decision's outputs With supply vector $\boldsymbol{s}$ estimated, the sourcing problem equation can be solved by plugging it in eq. (6.21). For each process type, the decision outputs can be calculated using eq. (6.22) - (6.24). It is important to note that demand $\boldsymbol{y}$ is not necessarily satisfied since decisions are based on available resources. For this, equation (6.25) calculates the unsatisfied quantity.

$$\boldsymbol{A}(\sum_{j}^{d} \boldsymbol{e}_j \boldsymbol{e}_j^T)\boldsymbol{s} = \gamma(j,d) \tag{6.21}$$

$$\gamma(1,n) = \gamma_{prod} \tag{6.22}$$

$$\gamma(n+1,n') = \gamma_{stor} \tag{6.23}$$

$$\gamma(n'+1,m) = \gamma_{supp} \tag{6.24}$$

$$\gamma(1,m) - \boldsymbol{y} = \gamma_{miss} \tag{6.25}$$

A comprehensive exemplification and explanation of *actions boundary*, *decision space*, and *operational configuration* in a STS can be found in section 6.4. Moreover, a numeric example is also presented to show the use of these mathematical elements in practice in section 6.5.

6.4 A graphical exemplification of a STS and AFRICA framework

Although products, processes, *actions boundaries* and *decision space* are labels arbitrarily defined for this framework, they are strongly rooted on elemental notions of the supply-chain model and its graph representation [4]. In this sense, it is also possible to derive this notions from a graph model of a STS. For instance, lets first imagine a fishmeal producer agent, ω_1, that resides in an simulation environment along with an identical fishmeal producer, ω_3, a fishmeal trader, ω_2 , and a market proxy-agent representing a global market of fish and gas (see Fig. 6.3a). Each producer agent is capable of capturing fish and manufacturing fish-meal by using gas as energy source for the fishing vessels and the heating of the boilers, respectively. The three agents possess a warehouse each that can be used to store finished goods or raw materials (see Fig. 6.3b). Trader agent ω_2, which is not involved in any production process, it is still involved in the SN since it is capable of buying and re-selling fishmeal and fish.

For the sake of demonstration, we can present the system as the composition of social and technical layer. In this sense, lets assume that the social links existing at that time-step t are represented by an interaction network (see Fig. 6.3a). In this network, interactions mainly occur due to transactions, and transactions yield to flows of money, information and products. We can say that the acquisition of products is the main driver of interactions and products are

[4]The system's graph representation is not novel in the LCA community, but we build our concepts on top of the representation proposed by Mutel, 2017, that treats products and processes as nodes, and exchanges as edges

the main assets that flow in a SN. In this network, the products are fishmeal, fish and gas (i.e., $P := \{Fishmeal,\ Fish,\ Gas\}$ and $n = 3$) Lets now assume that agent ω_1 can supply a certain demand of fishmeal by relying on a system depicted in a technological network (see Fig. 6.3c). In this network, edges represent flows of products that go from a product node to a process node and viceversa.

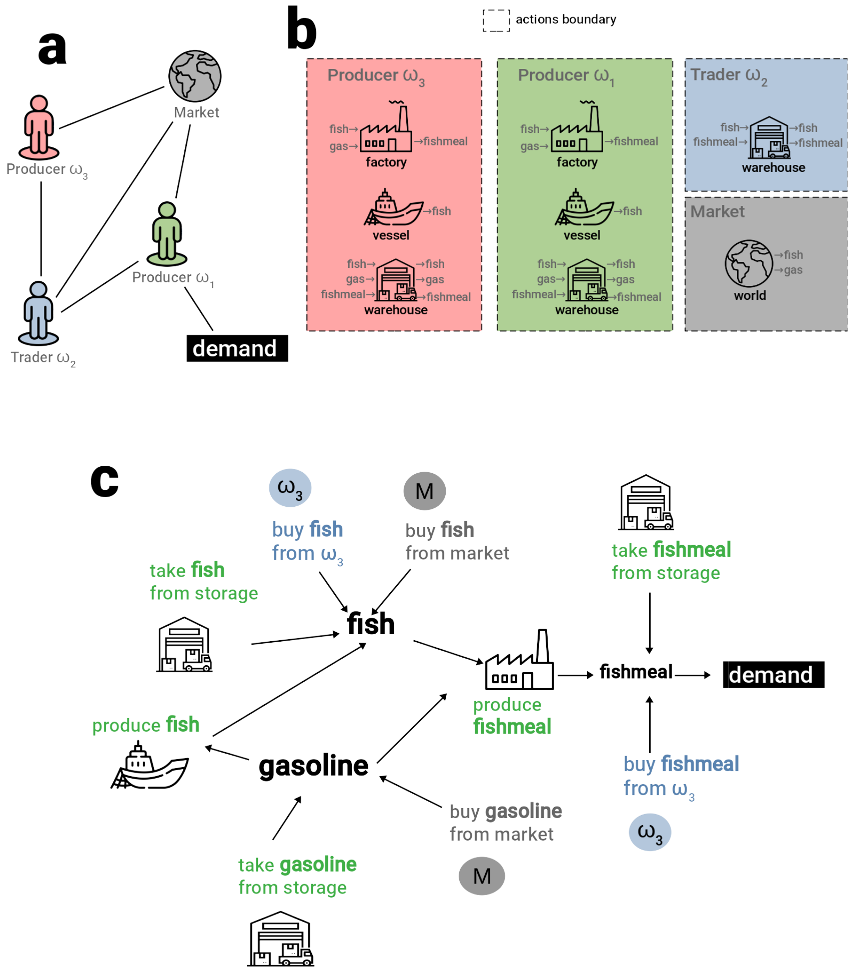


Figure 6.3: Different layers of a STS: (a) Interactions network among agents. (b) Boundaries of actions (c) Decision space of a specific agent

In this case, the set S_{ω_1} contains 9 processes (i.e., $|S_{\omega_1}| = 9 = m$), meaning that it represents all the possible processes that agent ω_1 can consider for supplying a given demand of fishmeal. This is equivalent to the *decision space*, previously defined. Finally, the *actions boundaries* of an agent ω_1 encompass the elements (e.g., plant, storage, vessel) that depend exclusively on agent's will (i.e., coloured frames in Fig. 6.3b). Moreover, this distinction can be clearly noticed when observing the agent ω_1 *decision space*, where processes' colour indicate belonging to a corresponding *actions boundaries.* This means that, despite being encompassed in the same the *decision space*, some processes are also dependent on other agents' actions.

6.5 Using AFRICA in a numeric example

The mathematical elements and equations proposed in AFRICA are meant to be used as part of different decision mechanisms, and they will be called and modified by every agent multiple times during run-time. To illustrate this, we provide a small numeric example where we use ω_1 (see Fig. 6.3c) and its *decision space* to illustrate how our framework is used to perform the calculations as part of an action mechanism. We use the "request for supply" as action mechanism depicted in Fig. 9.3b. The scheme starts with receiving a request for supply (i.e., (1) in Fig. 6.4) from a buyer that has a demand expressed in vector $\boldsymbol{y}$. The supplier agent will then use the operational configuration $\boldsymbol{\theta}$ and demand $\boldsymbol{y}$ to plug them into eq. 6.2 to calculate s by minimizing eq. 6.3 (i.e., monetary optimisation). Using eq. 6.21 - 6.25, the agent can determine how much quantity of each product can be supplied from production, from stocks, or how much is required to be purchased. The rule we impose for this example is that stocks should always be sold first, meaning that κ^f will be used instead of κ. In this sense, if there is enough stock, the supplier will immediately respond the supply request (i.e., (1) $\rightarrow$ (2) in Fig. 6.4) by delivering the product. When there is not enough demanded products in any storage facility, but there are enough inputs for its production, the agent will consume the inputs, produce the outputs, and deliver the demanded products (i.e., (1) $\rightarrow$ (5) $\rightarrow$ (2) in Fig. 6.4). In the absence of products in stock to deliver or to produce, the agent will evaluate other sourcing alternatives. Once again, using $\boldsymbol{s}$, the agent determines the products that will be obtained from production, from storage selection, and from purchasing processes, respectively. The agent will then send purchase requests to each one of the suppliers until the amounts indicated in $\boldsymbol{s}$ are obtained. If a supplier cannot or refuses to sell the product, the agent will update its beliefs and it will evaluate sourcing alternatives to submit again purchase requests in an iterative manner (i.e., (1) $\rightarrow$ (3) $\rightarrow$ (4) in Fig. 6.4). Once purchasing of all goods is possible, agents will pay and store them to then transform them into the final outputs (i.e., (1) $\rightarrow$ (3) $\rightarrow$ (5) $\rightarrow$ (2) in Fig. 6.4).

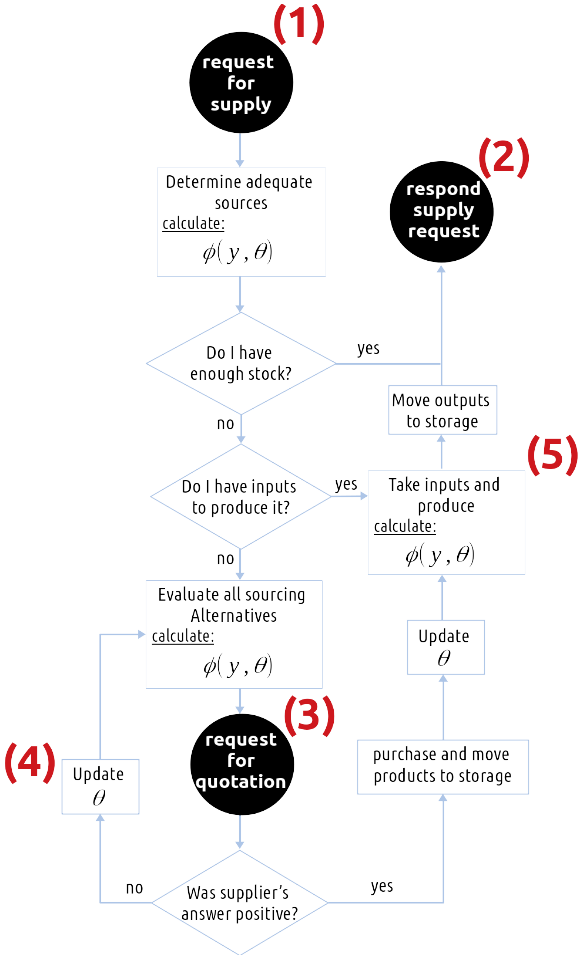


Figure 6.4: Flowchart depicting the decision scheme of an agent receiving a request of supply.

As it can be shown, agents can calculate $\boldsymbol{s}$ multiple times as part of an action mechanism. At any instant, agent's operational configuration, θ, can resemble the matrices and vectors shown in Fig. 6.5. When we use θ to evaluate sourcing alternatives (i.e., solving eq. 6.2 via monetary optimisation) using the *operational configuration* shown in 6.5, the resulting supply vector $\boldsymbol{s}$ looks like eq. 6.26. Here, $\boldsymbol{s}$ indicates that 50 units of fishmeal will be produced while the other 50 will be obtained from the storage number one. Moreover, 125 units of fish will be produced, 30 and 10 will be taken from storages number one and two, respectively, and 35 will be purchased from supplier ω_3. Finally, 67.5 units of gas will be purchased from the market of gas.

A

	produce FM (1)	produce fish (2)	produce gas (3)	take FM – storage (1) – ω_1 (4)	take fish – storage (1) – ω_1 (5)	take gas – storage (1) – ω_1 (6)	take fish – storafge (2) – ω_1 (7)	buy fish – ω_3 (8)	buy fish – market fish (9)	buy gas– market gas (10)	y	$z_\$$
FM 1	1	0	0	1	0	0	0	0	0	0	100	999
fish 2	-4	1	0	0	1	0	1	1	1	0	0	
gas 3	-0.1	-0.5	0	0	0	1	0	0	0	1	0	

F

	1	2	3	4	5	6	7	8	9	10	κ^{e}	κ^{f}	κ	c
production capacity 1	1.5	0.2	0	0	0	0	0	0	0	0	0	1	1	100
taking FM – storage (1) ω_1 2	0	0	0	1	0	0	0	0	0	0	2.6	0	2.6	50
taking fish – storage (1) ω_1 3	0	0	0	0	1	0	0	0	0	0	0.65	0	0.65	30
taking gas – storage (1) ω_1 4	0	0	0	0	0	1	0	0	0	0	0.2	0	0.2	0
taking fish – storage (2) ω_1 5	0	0	0	0	0	0	1	0	0	0	0.65	0	0.65	10
buying fish - ω_3 6	0	0	0	0	0	0	0	1	0	0	0	0.67	0.67	40
buying fish - market fish 7	0	0	0	0	0	0	0	0	1	0	0	0.69	0.69	∞
buying gas - market gas 8	0	0	0	0	0	0	0	0	0	1	0	0.2	0.2	∞

Q^{e}

CO_2-eq	0.3	0.15	0	0	0	0	0	0	0	0

Q^{f}

CO_2-eq	0	0	0	0.65	0.17	0.1	0.17	0.15	0.16	0.1

Q

CO_2-eq	0.3	0.15	0	0.65	0.17	0.1	0.17	0.15	0.16	0.1

Figure 6.5

$$s = [50, 125, 0, 50, 30, 0, 10, 35, 0, 67.5] \tag{6.26}$$

If we decide to obtain $\boldsymbol{s}$ using an environmental minimization, as shown in eq. 6.10, the result will be shown in eq. 6.27. We observe that the decision is now different if compared with the previous decision (eq. 6.26). While the agent is still producing 50 units of fishmeal and taking 50 from the storage, the fish is no longer produced by the agent, but bought from suppliers ω_3 and the fish market. Since no production of fish is required, the purchased gas will be less than the previous case. This numeric example can be replicated using the code in the repository (see section 13)

$$s = [50, 0, 0, 50, 0, 0, 0, 40, 160, 5] \tag{6.27}$$

Chapter 7

pacha: a python ABM toolkit for simulating supply networks in sustainability research

7.1 Introduction

This section provides a brief description of the pacha software. pacha is an operational toolkit that encapsulates the conceptual development presented in section I, and that contains the computational implementation of the elements presented in the AFRICA framework. Since we follow a paradigm in which agents are designed as socio-technical entities, AFRICA was a keystone in providing a mathematical framework to represent them. pacha is a python package developed to facilitate the coding and preparation of agent-based models in the context of sustainability research. The pacha engine is responsible for performing calculations and operations under-the-hood, so the practitioner can focus on the modelling of behaviors and systems. The outcome of pacha are agents' states accounted during the dynamic simulation, from which additional information can be derived, such as life-cycle inventories.

In the ecosystem of computational tools, life-cycle inventories can be dynamically obtained using different methods such as dynamic LCA (Pigné et al., 2019), digital twins (Boje et al., 2023), or coupled ABM-LCA (Marvuglia et al., 2022). However, the main distinction among them relies on their location in the technological-social spectrum. For instance, in a dynamic LCA the attention is on the technological flows (see [1] in Fig. 7.1), while an ABM focused on the consumption side is also dynamic, but the scope is on the interactions of the social network of consumers (Koide et al., 2023) (see [8] in Fig. 7.1). We locate the pacha user's need in the middle of a fully technical and a fully social model, but with a need of a fully dynamic approach. In this context, we start describing the current approaches used for ABM in sustainability research in section 7.2 to then present the scheme in which pacha operates 7.3.

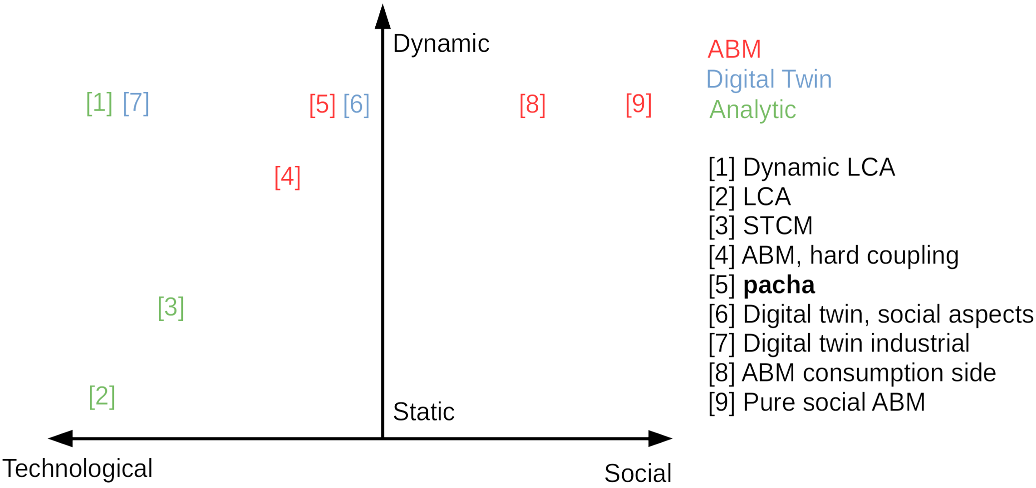


Figure 7.1: Ecosystem of computational approaches used in the modelling of life-cycle inventories for sustainability.

7.2 Current approaches in ABM for life-cycle inventory modelling

In inventory modelling, practitioners' goal is to solve an accounting problem that consist in calculating the flows that are provoked by a demand vector in a graph model of a supply chain. If the model depicts a technical system, the graph can be considered as static and the solution of the accounting problem can be obtained analytically using eq. A.2 in a single step and without the need of any other methodology (see section 3.3.4). If the system is modeled as a socio-technical system, the full graph is the composition of a static technological subgraph and a dynamic socio-technical subgraph. For this, implementations shown in the literature commonly involve modular approaches in which the results of the ABM instance are reformatted and fed into an LCA instance for impacts calculation during simulation (Baustert & Benetto, 2017; C. Davis et al., 2009; Micolier et al., 2019). Since the dataflow between instances is not necessarily unidirectional, practitioners have designed different pipelines depending on the agents behaviors and model assumptions.

7.3 A flexible simulation environment

pacha is programmed to simulate hard-coupling ABM-LCA models because. It provides a simulation environment capable of handling the communication among agents and the calculation of impacts at the same run-time (Baustert & Benetto, 2017; Micolier et al., 2019). Since impacts (i.e., or environmental flows) are attributes of the agents, these can be exchanged to each other as information for decision-making (see section 9). pacha can be used as an out-the-box toolkit since no additional data flows are required once a simulation is set up. Moreover, since it is written in python, practitioners can couple it with other types of computational models (see section 10). The smallest units are called agents, which inherit from a `pacha.engine.Agent` class. These agents are built as a combination of a collection of arrays representing its operational configuration, and a set of actions that control their behaviors. `pacha.engine.Agent` is programmed such that the user will rarely manipulate the arrays since most of the required manipulations can be done by agent's actions. All agents are part of a graph, which is an instance of a `pacha.engine.databases.AgentsDB` class designed to be an in-memory container of the agents. This, at the same time, is contained in a simulation environment, which is an instance of `pacha.engine.Simulator`. The simulator contains an environment entity that can be used to modify the state of any agent (see section 10). Moreover, the simulator is also responsible for scheduling agents' actions and recording all the states as data in a structured database. The simulator is contained in a scenario runner which is an instance of `pacha.tools.ScenarioRunner` class. The simulator is designed to operate in full isolation of the rest of the modules, meaning that it can be serialized. In this sense, the scenario runner can operate multiple instances of the simulator in parallel by feeding different parameters each time. pacha is programmed to prepare the tasks and to operate in chunks so the created data is manageable when the number of parallel simulations increase. The above mentioned components are shown in 7.2.

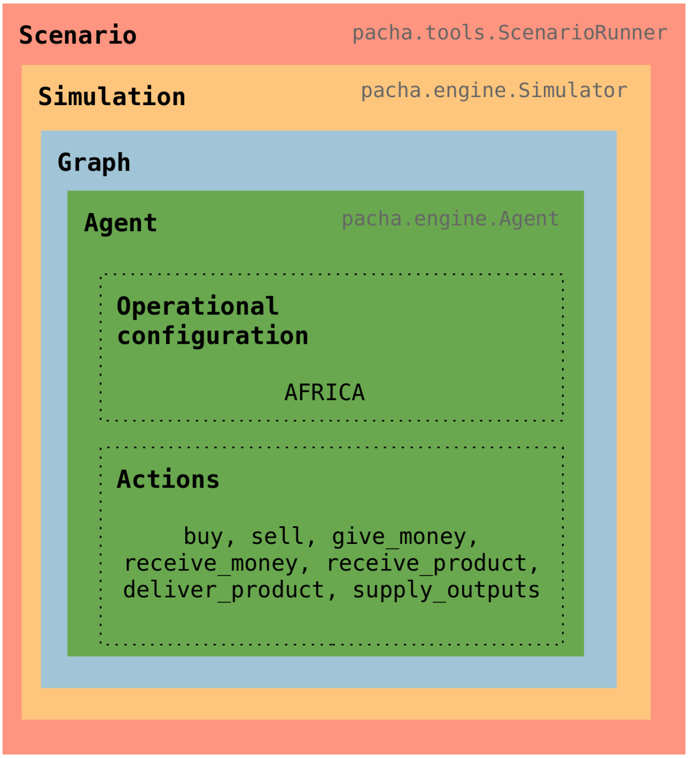


Figure 7.2: Structure of a simulation using pacha.

7.4 Using pacha

Minimum four files are the required by pacha to start a simulation: `rules.py`, `instructions.py`, `schemes.py`, `parameters.yaml`. The `rules.py` contains the custom meta-agents that have been programmed by the user. These inherit from `pacha.engine.Agent` class, and must contain a `run()` and a `wake_up()` functions that will be called during a simulation time step (see them in use in section 10). The `instructions.py` file should contain all the instructions that the simulator or the environment must perform before, during, and after the simulation. For instance, when modelling a market system, exogenous changes in price will be defined as functions in this file. `schemes.py` can be used to define default actions that are meant to override the default ones provided by pacha (e.g., giving money, requesting a quote, etc.). Finally, the `parameters.yaml` contains all the parameters described in an human-readable yaml format (Brian Ben-Kiki et al., 2005) that will be consumed by the simulator.

A user will require an interactive development environment to program the model using python syntax. For instance, in the example shown in Fig. 7.3, the `rules.py` contains a meta-agent class called "cookie_plant_rules" which inherits from the `pacha.engine.actions.ProducerActions` class. This means that, when instantiated, an agent of this class will have all the methods contained in a default `pacha.engine.actions.ProducerActions`. In the example, the agent first observes the stock and demand of cookies and stores them in the `stock` and `demand` variables, respectively. It then executes its rules that can understood as follows: "if the `stock` decreased below 30 percent of the `demand`, then make request quotes to all your suppliers, and then produce `demand` units of cookies."

rules.py | schemes.py | instructions.py | parameters.yaml

```python
from pacha.engine.actions import ProducerActions

class cookie_plant_rules(ProducerActions):

  def run(self):

    stock = self.properties.products["cookie"].stock
    demand = self.properties.products["cookie"].demand

    if (stock < demand * 0.3):

      self.schemes.Production.quote_update_all_inputs()
      self.supply_outputs("cookie", demand)
```

Figure 7.3: Example of code used when modelling an agent using pacha.

This scheme of programming agent is strongly leveraged on the computational structure of AFRICA, which treats agents as elements with inputs and outputs. Because of this, the operational configuration is programmed as a set of array objects using highly efficient low-level libraries (e.g., numpy and scipy) (Harris et al., 2020). Finally, while it is fully operational, pacha is a project under current development to be released as an open-source package.

Chapter 8

Summary Part II

Part II represents the core of the methodological development of this thesis. On the one hand, AFRICA was proposed as an algebraic, flexible, and language-agnostic framework for modelling socio-technical agents. On the other hand, pacha is a practical application of the conceptual development presented in section I, and the computational implementation of AFRICA. This process of thought can be visually represented in Fig. 8.1. We aimed for an operational methodology that could allow us to model a socio-technical system. Such methodology would have to rely on principles, and it would require a framework designed for ABM. This operational methodology was an operational software compatible with the ABM paradigm: pacha.

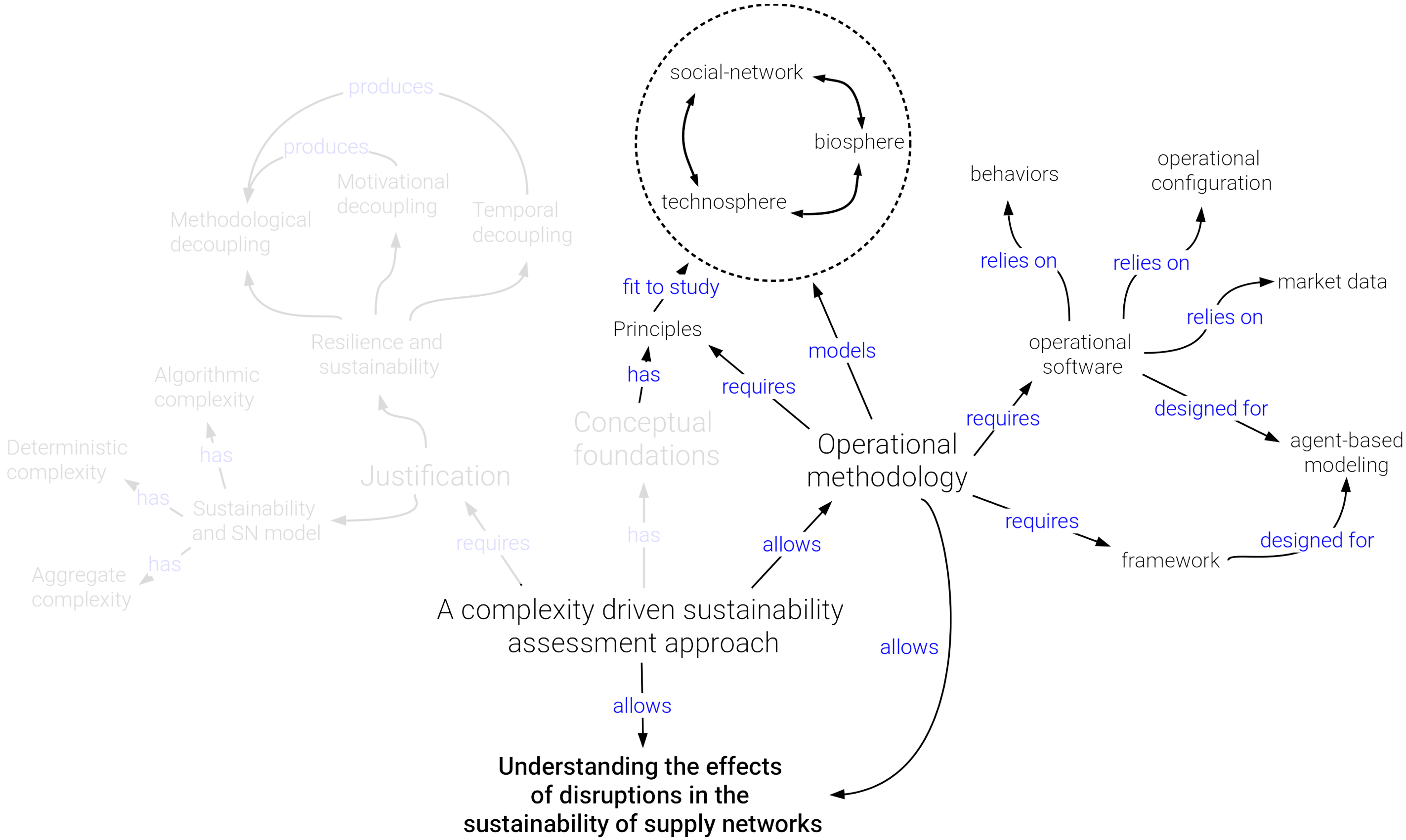


Figure 8.1: Expanded conceptual map of the aspects developed in chapter II

Part III

Hands on AFRICA: two cases of study

Chapter 9

Exploring fundamental questions of sustainable agents and systems

List of symbols

D_c Total consumers demand.

T Total time steps of a simulation.

$U_{\omega,t}$ Utility of the decision taken by agent ω in a time step t (consumers).

V_o Default perceived value of the product (consumers).

$Vf_{\omega,t}$ Product's perceived value, from an agent ω in a time step t (consumers).

Ω_c Set of consumer agents.

Ω_p Set of producer agents.

Ω_w Set of wholesaler agents.

Ω Set of agents composed by producers, consumers and wholesalers.

ω Any agent, where $\omega \in \Omega$.

τ Number of Montecarlo simulations.

aoc_ratio Percentage of Agents of Change.

$att_{\omega,t}$ Attitude of an agent ω in a time step t (consumers).

$cost_o$ Initial cost of a unit product (producers).

d_p Daily demand for any producer.

f_d Demand increase factor.

f_{exp} Daily expense factor.

f_{lack} Lack of capacity factor.

f_{profit} Expected profit of a unit of product (producers).

$norm_{\omega,t}$ Business norm of an agent ω in a time step t (consumers).

$sell\_ratio$ Percentage of producers directly connected to wholesalers.

t_b Days until bankruptcy.

t Specific time step.

$variation\_ratio$ Scale parameter used in a log-normal distribution to add variability to the environmental performance of agents(producers).

9.1 Introduction

To demonstrate the utility of AFRICA, we propose a toy SN model in which we explore the consequences of the gradual introduction of agents with sustainable attitudes. The effect of sustainable behaviors is an ongoing topic of interest and identifying key factors and potential opportunities of action is relevant for an adequate policy-making (J. Li et al., 2020; Wang et al., 2018; Yang et al., 2022). More specifically, policies are now not only oriented on improving the productive system, but also on promoting green consumption as a pro-environment and altruistic behavior to be adopted by consumers as part of their process of value selection and satisfaction of needs (Mainieri et al., 2010; Rustam et al., 2020; Yang et al., 2022). This change in consumers' behaviors is meant to benefit companies with a sustainable business norm, promoting, implicitly, the adoption of a new mentality among suppliers. For suppliers, adopting a green behavior can be interpreted as the prioritisation of sourcing alternatives and technologies that minimise the environmental burden of the production. In this sense, it is important to first determine if the change in individual attitudes will represent an advantage or disadvantage for the agents, and if the system will effectively change in the desired direction.

The principle for companies is that successful business interactions with suppliers enables the production of tradable goods to then allow the generation of revenue. Revenue is generated only when successful relationships with clients are established, being clients responsible for selecting a supplier based on their business norm. In an SN where most companies follow a profit-driven business norm, the adoption of green behaviors can be interpreted as transgressive to the common notion of business' objectives, meaning that we can label these hypothetical norm-transgressing companies as Agents of Change (AOCs). Since an AOC should be more likely to report less environmental impacts, it should also have a higher likelihood to be selected if the client shares the same sustainable business norm (i.e., compared to a profit-driven agent). In this sense, it is logical to propose the following conjecture:

Conjecture 1 *The financial survival of a company depends on the "business norms" of its clients, therefore the financial survival likelihood of an AOC should be related to the number of companies in the SN following the same business norm.*

This conjecture can be studied as two specific questions: 1) is an AOC always in disadvantage when adopting a sustainability-driven business norm in a system dominated by profit-drive agents?, and, 2) how much does the system improve (e.g., increase added value, decrease environmental burdens) from this behavioral change? We delved into the study of these questions by conducting a series of experiments in which the goal was understanding the financial survivability of companies given the adoption of a determined business norm under different scenarios. In this study, we define financial survivability as the "capacity of a company to fulfill their financial objectives in a given period before reaching bankruptcy"[1]. For this, we progressively introduced AOCs in an SN composed by producers, wholesalers and consumers in an ABM model where agents were programmed relying on the mathematical elements presented in AFRICA. We proposed two scenarios in which we assumed different mechanism of appearance of AOC: random and systematic. For the first scenario (a), AOCs appear randomly in the production network, while for scenario (b), they appear in the first layer of suppliers which is the closest to the wholesalers and, consequently, to the consumption network (see Fig. 9.2b). Each scenario consisted in the computation of Montecarlo simulations where the proportion of AOCs was gradually increased from 0% to 100%, $\tau = 100$ times each, (i.e., different random-state) during $T = 40$ days. The effect of the introduction of this new business norm was evaluated by the change of the probability of an agent to go bankrupt given the decision of becoming an AOC (i.e., $P(B|AOC)$). The selection of $T = 40$ and $\tau = 100$ responds to the system equilibrium state reached after $T = 35$, and the convergence of average of the Montecarlo simulations after$\tau = 100$, respectively (see section 9.4). In the first case, equilibrium makes reference to the state during a simulation in which a particular statistic (i.e., average product impact) becomes stationary. Identifying the time step in which this equilibrium is reached helps to avoid unnecessary computation since any new information does not change the analysis outcome. In the second case, convergence makes reference to the state from which one additional simulation does the variance of a particular statistic (i.e., systems emissions and money accumulation).z4

9.2 modelling of the SN

9.2.1 Formulation of the production-consumption model

We proposed a parametrized SN model in which the total demand D_c was endogenously generated by the consumer side, and supplied by the wholesalers and the producers following a push strategy (see Fig. 9.1(a)). In a push system, agents start production on the basis of a forecasted demand that is expected to be pushed until reaching the consumer. For the toy model we set a pool of $|\Omega| = 202$ agents composed by 100 FM producers, Ω_p, 100 fishmeal consumers, Ω_c, and two wholesalers, Ω_w. The expected demand was $1 + f_d$ times higher for the wholesalers and $1 + {f_d}^2$ times higher for the production side, being f_d the demand increase factor. The expected demand of each producer agent was a fraction $(sell\_ratio \times \mid \Omega_p \mid)$ of the total expected demand for the production side, being $sell\_ratio$ the fraction of producers directly connected to the wholesalers, and $\mid \Omega_p \mid$ the amount producers agents. Production agents aimed to satisfy a daily demand d_p based on its production capacity, which was constrained by the factor f_{lack}. Producer agents were provided with an initial amount of money which represented the expected daily profit $d_p * f_{profit} * cost_o$ that could be received

[1]We propose this concept by leveraging on a similar notion proposed by Ivanov, 2020 where the concept of viability is used in survival-oriented study of disruptions

during t_b days. In this case, f_{profit} refers to the expected profit per unit of product, while $cost_o$ is the initial cost of production. The bankruptcy mechanism is set by fixing a daily expense that is a fraction f_{exp} of the expected daily profit. Finally, producers made profit from sales by transforming gas and raw fish into fishmeal, which are inputs obtained from two market proxy-agents that behave as unconstrained suppliers (see Fig. 9.1b).

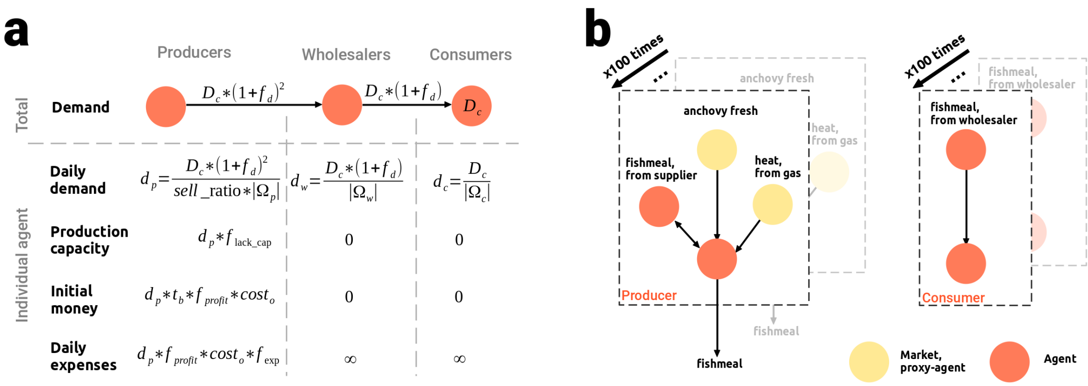


Figure 9.1: Parameters that control the demand and influence agent's bankruptcy condition (a). Graphical representation of a producer connected to one supplier and a consumer connected to one wholesaler (b). Parameters: Ω_p= set of producers, Ω_w= set of wholesalers, Ω_c= set of consumers, D_c= consumers demand, f_d= demand increase factor, d_p= producer daily demand, $sell\_ratio$=fraction of producers connected to wholesalers, f_{lack}= lack of production factor, t_b= days before bankruptcy, f_{profit}= profit factor, $cost_o$= initial forecasted cost, f_{exp}= daily expense fraction

Regarding the topological characteristics, the production network possesses scale-free properties and it is randomly generated using the Barabási-Albert generation model (Albert & Barabási, 2002) (see Fig. 9.2a). This model has been widely used for generating networks with degrees that follow a power law distribution, which is a property observed in many real world SN (Fan et al., 2022; Zhao et al., 2019). Market proxy-agents' were built as mimics of ecoinvent 3.6 activities (Wernet et al., 2016) that were adapted to the AFRICA framework. The consumers network has small-world network properties that is generated using the Watts-Strogatz model (Watts & Strogatz, 1998) (see Fig. 9.2a). Consumers are modelled as socio-technical agents without production processes that demand fishmeal from the wholesalers (see Fig.9.1b). These agents do not produce emissions and they can become AOC using the green behavior diffusion model presented in (Yang et al., 2022). This behavior diffusion model considers the behavior of the neighboring consumers and it is detailed in the following section.

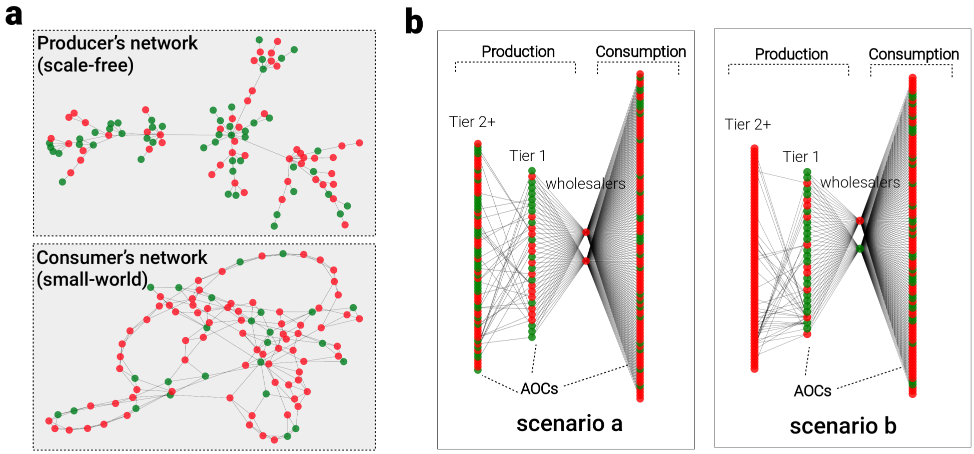


Figure 9.2: Graphical representation of the topologies used in the producer and consumer networks (a). Multipartite representation of the complete network of agents composed by a combination of scale-free and small-world networks for the two proposed scenarios (b). Red nodes depict profit-driven agents and green ones represent AOCs

9.2.2 Diffusion of the green behaviour

Consumers' decision scheme is different from the one used for producers since it is based on the green consumption model proposed by Yang et al., 2022. In this model, at a given time step t, a consumer ω will choose a consumption norm $norm_{\omega,t}$ depending on the state of three components: consumer's attitude $att_{\omega,t}$, perceived value $Vf_{\omega,t}$, utility of the decision $U_{\omega,t}$. $att_{\omega,t}$ indicates the negative or positive (i.e., 0 or 1, respectively) perception that a consumer has towards being sustainability-driven, while perceived value $Vf_{\omega,t}$ is a quantifiable and relative indication of the superiority of buying from a green wholesaler over a normal wholesaler.

$att_{\omega,t}$ and $Vf_{\omega,t}$ are inner beliefs that can be affected by endogenous drivers or external influences. On the one hand, attitude $att_{\omega,t}$ is endogenously modified when the current perceived value $Vf_{\omega,t}$ surpasses the perceived value of buying from a normal wholesaler or default perception V_o. On the other hand, this attitude is externally modified when neighbours' attitude (i.e., average) surpasses a determined threshold (e.g., more than fifty percent). Similarly, current perceived value can be influenced by the perception shared by neighbours with a positive sustainable attitude (i.e., weighted average). Being β a consumer agent in $\Omega_c \backslash \{\omega\}$, and $c_{\omega,\beta}$ the binary variable that indicates a connection or disconnection between ω and β, the rule that sets the values of $att_{\omega,t}$ and $Vf_{\omega,t}$ can be described in eq. 9.1 and eq. 9.2, respectively.

$$att_{\omega,t} = \begin{cases} 1, \text{if } Vf_{\omega,t} > V_o \\ 1, \text{if } \frac{\sum_\beta c_{\omega,\beta} \times att_{\beta,t}}{\sum_\beta c_{\omega,\beta}} \geq 0.5 \\ 0, \text{if } \frac{\sum_\beta c_{\omega,\beta} \times att_{\beta,t}}{\sum_\beta c_{\omega,\beta}} < 0.5 \end{cases} \tag{9.1}$$

$$Vf_{\omega,t} = \begin{cases} \frac{\sum_\beta c_{\omega,\beta} \times Vf_{\beta,t} \times att_{\beta,t}}{\sum_\beta c_{\omega,\beta} \times att_{\beta,t}}, \text{if} \sum_\beta c_{\omega,\beta} \times att_{\beta,t} > 0 \\ V_o, \text{if} \sum_\beta c_{\omega,\beta} \times att_{\beta,t} = 0 \end{cases} \tag{9.2}$$

Net utility of the decision $U_{\omega,t}$ was originally composed by a combination of consumer's willingness to pay, benefit and total cost (W. Li et al., 2018; Yang et al., 2022), nevertheless, we used a simplified version in which benefit and other parameters (e.g., subsidies, green costs, information search cost, etc.) were not considered (see eq. 9.3). In eq. 9.3, W_o represents a basic willingness to pay and w the additional amount that consumers are willing to pay per additional of increase in perceived value $Vf_{\omega,t}$. $Cost$ represents the cost of the product at time step t as provided by the supplier.

$$U_{\omega,t} = W_o + (Vf_{\omega,t} - V_o) * w - Cost_t \tag{9.3}$$

Finally, consumption norm $norm_{\omega,t}$ is a binary variable that indicates if the consumer will be cost-driven (i.e., cost minimization) or sustainability-driven (i.e., environmental minimization). This norm depends on the current attitude $att_{\omega,t}$ and the utility of purchasing a green product $U_{\omega,t}$ (see eq. 9.4). One of the two wholesalers will be an AOC responsible for selecting the products with the lowest impact (i.e., environmental minimization). In this sense, consumer can opt for a regular product or a sustainable one by deciding between the two wholesalers.

$$norm_{\omega,t} = \begin{cases} 1, \text{if } norm_{\omega,t-1} = 1 \\ 1, \text{if } norm_{\omega,t-1} = 0 \text{ and } att_{\omega,t} = 1 \text{ and } U_{\omega,t} > 0 \\ 0, \text{else} \end{cases} \tag{9.4}$$

9.2.3 Model setup and simulation conditions

All producer agents are initially created as profit-driven, but we modified the business norm of a percentage *aoc_ratio*. Producers can sell and purchase fishmeal among themselves if a business connection exists, but only a percentage of them *sell_ratio* (i.e., 0.3) are selected to be in the first layer of the supply side and connect to wholesalers. The selection of AOCs and seller agents are both independent processes, meaning that each agent has the same probability of being selected for each case. One of the wholesalers is initialized as an AOC, while the other is a normal profit-driven agent. While all producers are created as homogeneous agents, we added variability by modifying their environmental performance (i.e., Impacts matrix $\mathbf{Q}$). Each modified value is sampled from a log-normal distribution with a location parameter equal to the logarithm of the original value and scale parameter equal to *variation_ratio*. Agents initial operational configuration (i.e., matrices $\boldsymbol{A}, \boldsymbol{Q}, \boldsymbol{F}, \boldsymbol{k}, \boldsymbol{c}$, and $\boldsymbol{z}$) and model parameters were ingested using an Excel template and a `parameters.yaml` file, respectively.

9.2.4 Agents' action mechanisms

Agents act through different action mechanisms such as transforming, storing, selling, buying, or requesting and making quotations (see Fig. 9.3b). The rule that triggers the different action mechanisms is depicted in Fig. 9.3a, and it establishes that an agent will attempt to satisfy the expected demand only if its current stock drops under certain threshold (i.e., 80 percent). All rules, action mechanism, and the whole simulation environment were implemented using pacha, the python toolkit presented in chapter 7. In this sense, our final complete synthetic database was conformed by the daily final state of every agent for every simulation and scenario and every value of *aoc_ratio* (i.e., $|\Omega| \times \tau \times t \times 10$). Finally, for each scenario, the simulation followed the pseudo-code described in Algorithm 1.

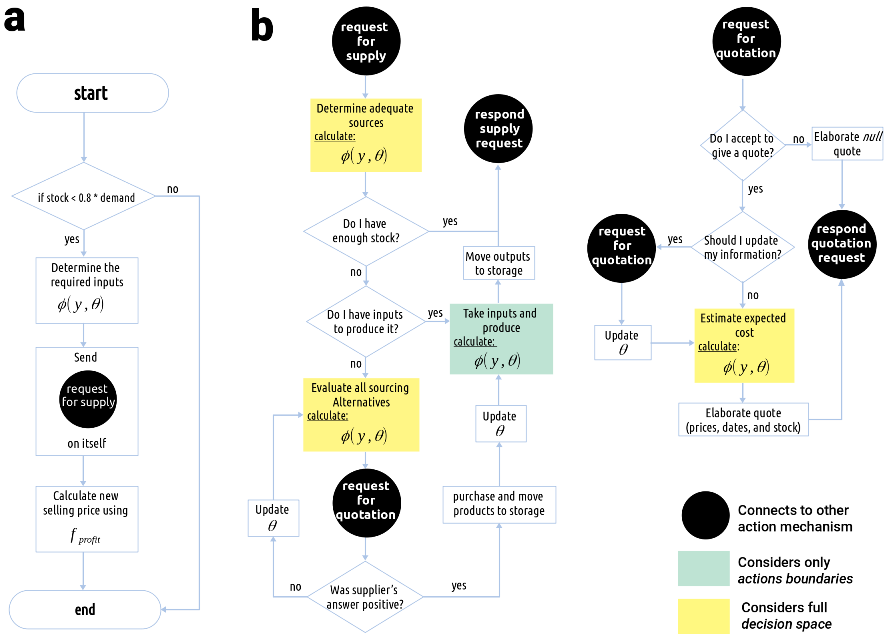


Figure 9.3: Main rule (a) that triggers different action mechanism (b) of a socio-technical agent that aims to maintain a constant stock of a product.

Algorithm 1: Simulation setup and experimentation for each scenario

Data: G := graph class, Ω := set of all agents, Ω_p := set of producer agents, Ω_w := set of wholesaler agents, τ := number of simulations, t := simulation days, aoc_ratio := ratio of AOC, variation_ratio := percentage of change in emission profile, sell_ratio := percentage of sellers, db := empty structured database

```
for sim ← 1 to τ do
    G_sim ← G( ) ;                                          // Creates new instance
    add wholesalers into G_sim
    initialise producers and add into G_sim ;               // uses Barabassi-Albert algorithm
    initialise consumers and add into G_sim ;               // uses Watts-Strogatz algorithm
    seller_agents ← sample |Ω_p| ∗ sell_ratio from Ω_p
    aoc_agents ← sample |Ω_p| ∗ aoc_ratio from Ω_p ;        // different for each scenario
    for agent ∈ Ω do
        initialise agent operational configuration ;        // ingests matrices A,F,B, etc.
        connect with market proxy-agents ;                  // uses ecoinvent 3.6 data
        agent.B = Lognormal(log(B), variation_ratio) ;      // scales each value in B_e×m
        if agent ∈ aoc_agents then
            agent.parameters.aoc ← True
        end
    end
    if producer ∈ seller_agents then
        for wholesaler ∈ Ω_w do                             // connects seller to wholesalers
            creates an edge from producer to wholesaler
        end
    end
    for consumer ∈ Ω_c do                                   // connects consumer to wholesalers
        creates an edge from consumer to wholesaler
    end
    for day ← 1 to t do
        shuffles order in Ω ;                               // avoids undesired deterministic behaviour
        for agent ∈ Ω do
            agent.run() ;                                   // agent uses programmed rules
        end
        for consumer ∈ Ω_c do
            consumer.diffuse() ;                            // runs a behaviour diffusion algorithm
        end
        record states, impacts, and useful information in db
    end
end
```

9.2.5 Parameters

As mentioned beforehand, every experiment consisted in Montecarlo simulations in which different parameters were varied depending on the evaluated aspect of the experiment. The stochastic parameters and components of the model are described Table 9.1, while deterministic parameters used in both scenarios a and b are shown in Table 9.2.

Stochastic parameters

Parameter	algorithm/distribution	description
$variation\_ratio$	log-normal	$loc = 0$, $\sigma = 0.5$, $seed = 0$
producer network	Barabási-Albert	$n = 1$, $seed = 1$
consumer network	Watts-Strogatz	$K = 9$, $P = 0.1$, $seed = 1$
$sell\_ratio$	Sample without repetition	$seed = 2$
aoc_ratio	Sample without repetition	$seed = 3$

Table 9.1: Stochastic parameters used in the montecarlo simulations

Deterministic parameters

Parameter	Value
f_{lack}	0.5
f_d	0.2
$sell\_ratio$	0.3
f_{profit}	0.2
f_{exp}	1
t_b	10
$cost_o$	0.84
D_c	800
aoc_ratio	[0, 1]

Table 9.2: Deterministics parameters used scenarios a and b.

The consumer diffusion model used the parameters described in Table 9.3.

Diffusion model parameters

Parameter	Value
V_o	1
β	2
w	3
Vf	5
$norm_o$	0.1
W_o	10
att_o	0.35

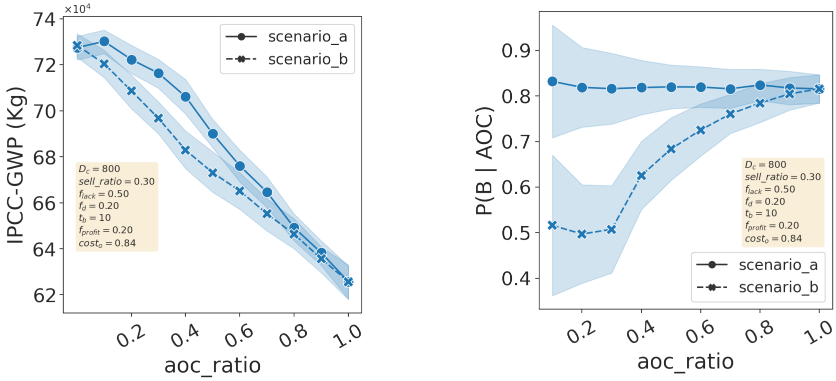
Table 9.3: Parameters used in the diffusion model. att_o : initial percentage of consumers with $att = 1$, $norm_o$: initial percentage of consumer with $norm = 1$

9.3 Results

We accounted for daily life-cycle impacts and financial state of each agent, where the condition of "bankruptcy" was reached when agents' available money reached 0 (i.e. $\boldsymbol{z}_{\$} \leq 0$). Results indicate that in both scenarios, the progressive introduction of AOCs yields to a progressive reduction of GWP impacts until reaching a reduction of approximate 13 percent when $aoc\_ratio = 1$ (see Fig. 9.4a). In the case of scenario a, this reduction happens in a non-monotonic fashion since there is an increase in impacts when $aoc\_ratio = 0.1$. aoc_ratio values of 0 and 1 represent the trivial cases where all producers have the same business norm, which is why the impacts are the same for both scenarios. However, when aoc_ratio is between 0.2 and 0.5, scenario b clearly shows a higher reduction in impacts compared to scenario a (see Fig. 9.4a).

Regarding financial performance, results for scenario a indicate that the probability of going bankrupt given being an AOC stays around 0.82 on average regardless of the aoc_ratio (see Fig. 9.4b). However, the multiple Montecarlo simulations showed that this probability ranges from 0.7 to 0.9 when $aoc\_ratio \leq 0.3$. For the case of scenario b, the conditional probability remains around 0.51 for aoc_ratio values between 0.1 and 0.3, and then it increases in a logarithmic fashion until converging to 0.82 (see Fig.9.4b). Similarly to scenario a, the Montecarlo simulations show that the conditional probability varies from 0.35 to 0.65 with $aoc\_ratio \leq 0.3$ (i.e., less than 0.3) to then converge to a stable variance after reaching a threshold of $aoc\_ratio = 0.3$. The appearance of this threshold can be explained by the selection of $sell\_ratio = 0.3$, since in this case all of the AOCs are contained in the group that supplies the wholesalers. For cases where $aoc\_ratio > 0.3$, AOCs in the first tier of suppliers have a beneficial effect that propagates to the remaining AOCs, explaining the buffered increase in the conditional probability.

It can be observed that in both scenarios, the conditional probability caps, on average, at 0.82. This occurs at any aoc_ratio value for scenario a, and when $aoc\_ratio = 1$ in scenario b. We can imply that this probability cap is the natural bankruptcy probability of the proposed SN, meaning that it is independent of the aoc_ratio value, and it is dependent on the production capacity, the daily expenses, the initial money, and the forecasted demand (i.e. f_{lack_cap}, f_{exp}, t_b, and f_d and D_c).

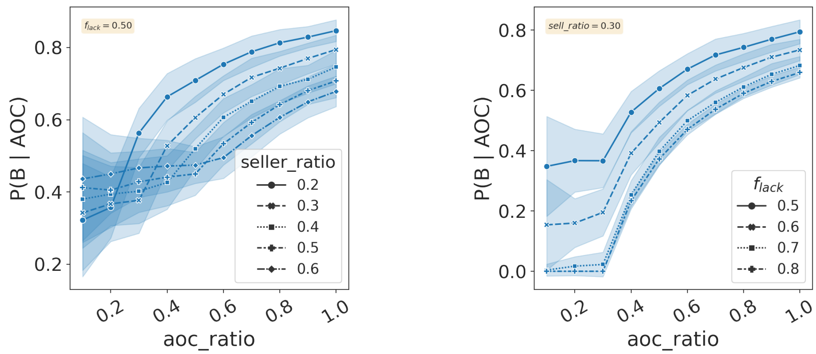


(a) (b)

Figure 9.4: Change in GWP impacts given the increase of AOCs for each scenario (a). Evolution of the probability of going bankrupt given the probability being an AOC for each scenario (b).

9.4 Sensitivity analysis

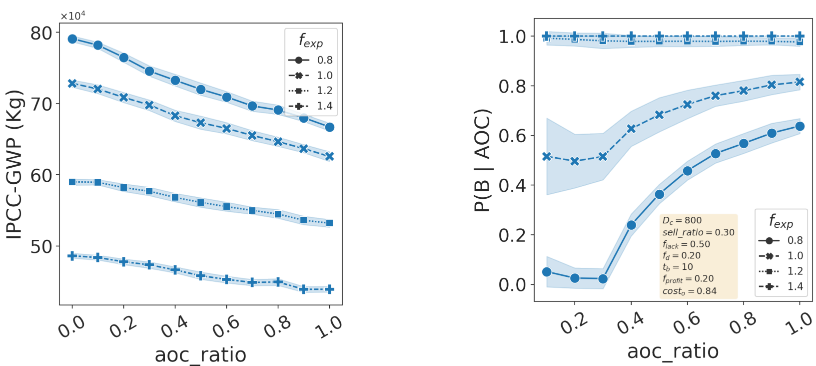
To address the sensitivity of the results to the $sell\_ratio$ parameter, we conducted multiple iterations of the experiment where we gradually varied this value from 0.2 to 0.6 (see Fig. 9.5a). We observed that, indeed, the before mentioned threshold appears when $aoc\_ratio = sell\_ratio$ and it separates two patterns: a constant and low probability trend (i.e., $aoc\_ratio \leq sell\_ratio$) and a logarithmic increase trend (i.e., $aoc\_ratio \geq sell\_ratio$). Similarly, we evaluated the sensitivity to the initial conditions by modifying the lack of capacity factor f_{lack}, from 0.5 to 0.8 (see Fig. 9.5b)). This factor is meant to reduce the producer's capacity to satisfy the expected daily demand. As it can be seen in Fig. 9.5b), the variation in f_{lack} shifts the conditional probability along the y-axis while maintaining the same dual-trend pattern. For $aoc\_ratio \leq 0.3$, this shift is, on average, in the range of 0 to 0.38; while for $aoc\_ratio = 1$, this range reduces to 0.63 to 0.79. From this, we can interpret that the patterns observed in scenario b persist regardless of the initial SN conditions and they indeed correspond to the systematic introduction of the AOC's.



(a) (b)

Figure 9.5: Variation of the $P(B|AOC)$ for different $sell\_ratio$ values (a) and different f_{lack} values (b).

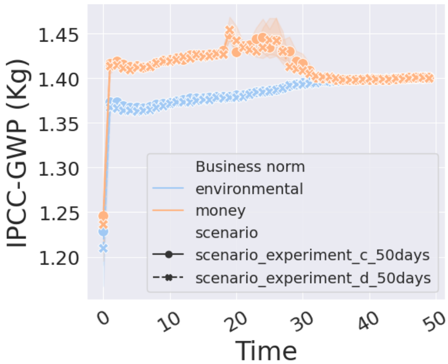
As previously described, the dual-trend pattern observed due to the introduction of systematic AOCs is independent of the initial conditions. This argument can be supported when evaluating the sensitivity of the model to changes in other parameters. Since the bankruptcy condition is determined by the daily expense and the capacity of generating revenue, we evaluated the impacts and the conditional probability for different values of f_{exp}. As we can see in Fig. 9.6a, the total impacts shift along the y-axis while maintaining the same trend. This occurs because by the end of the simulation, more agents go bankrupt the higher the value of f_{exp}, meaning that fewer products are produced. In the case of the conditional probability Fig. 9.6b, we observe that the dual-trend holds for low values $f_{exp} \leq 1$, while for higher values the probability is almost 1 since most agents will go bankrupt due to the excessive expenses.



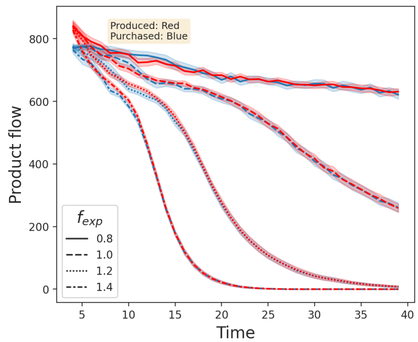
(a) (b)

Figure 9.6: Change in GWP impacts (a) and $P(B|AOC)$ (b) for different aoc_ratio and f_{exp}.

The effect that this parameter has over the bankruptcy of agents can also be shown in Fig. 9.7b, in which the daily production and consumption of fishmeal can be observed. It can be noted that the product flow decreases earlier in the simulation the higher the f_{exp} value. This can be explained by the quantity of agents that go bankrupt that are not able to keep producing goods. It can also be noted that at the beginning of the simulation the production (red line) is higher than the consumption (blue line) until reaching a point where the consumption matches the demand. Moreover, with respect to the life-cycle impacts of the products flowing along the SN, it can be noted that the impacts of goods sold by AOCs and profit-driven agents converge to an average of 1.40 Kg CO_2eq after 32 days for both scenarios. Again, this occurs because the number of producers reduces with time due to the initial conditions (see Fig. 9.7a).



(a)



(b)

Figure 9.7: Daily production of fishmeal (red) and daily its daily consumption (blue) for different f_{exp} (a). Evolution of life-cycle impact of the product sold by AOCs and by profit-driven agents (b).

To understand the relationship between the parameters of the SN model, we plotted the daily expenses surface for different values of *sell_ratio* and f_{exp} (see Fig.9.8). We observe that the daily expenses increase exponentially with low values of *sell_ratio* and high values of f_{exp}. Moreover, when including the initial money with $t_b = 2$ (blue line), we observe that it follows the same exponential trend as the daily expenses. This can be interpreted as a linear relation between the initial money and the daily expenses, meaning that the gap between them (i.e., the closer the agent is to bankruptcy) is also controlled by t_b.

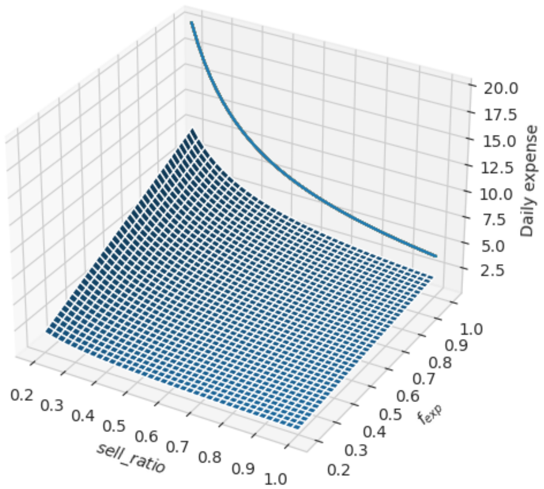
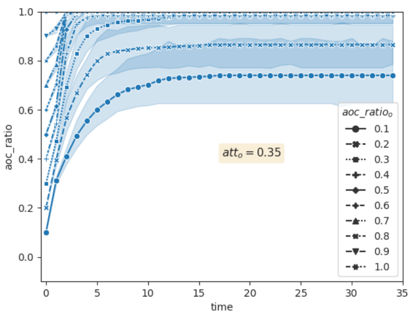
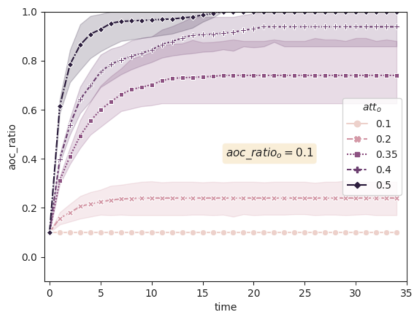


Figure 9.8: Daily expenses surface create by different *sell_ratio* and f_{exp} values. Blue line indicates the change in initial money when $t_b = 2$.

Finally, different parameters used for the diffusion model were explored to determine the evolution of the AOCs in the consumption network. As it can be observed, the model reaches equilibrium after 10 days regardless of the initial parameters. This can be explained by the amount of agents in the network and it justifies the selection of $T = 40$.



(a)



(b)

Figure 9.9: Evolution of the proportion of AOCs in the consumers networks due to the diffusion model. (a) shows the influence of the initial proportion of AOCs. (b) shows the influence of the initial proportion of consumers with $att = 1$.

Chapter 10

Understanding the sustainability of the fishmeal industry under the effects of disruptions

List of symbols

E Set of edges among agents.

$G(\Omega, E)$ Graph of agents in Ω connected by edges in set E.

T Total days of the simulation.

Ω^b Set of buyer agents.

Ω^m Set of market proxy-agents.

Ω^p Set of producer agents.

Ω^v Set of vessel agents.

Ω Set of all agents in a simulation.

ω An agent in the simulation.

ϕ Function that solves de sourcing problem and returns a supply vector s.

τ Number of Montecarlo simulations.

θ_ω Operational configuration of an agent ω.

θ_ω Operational configuration of an agent ω.

$allocation$ Fishmeal allocation factor.

$buyer\_demand$ Demand of fishmeal of given buyer countries.

$capacity^p$ Maximum anchovy processing capacity per hour.

$capacity^v$ Maximum capture capacity of a vessel.

$capture\_rate$ Factor that affects the capacity $capacity^v$.

$cost^v$ Production cost of a given unit of landed anchovy.

$decrease$ Percentage of the availability of anchovy that decreases due to a disruption.

$demand\_share$ Percentage of demand share corresponding to a given buyer country.

$disrupt\_rate$ Parameter that indicates the percentage of agents that may be affected by disruptions.

$disrupted_t^{\omega}$ Variable that indicates if an agent ω is disrupted at a time step t.

$disrupt$ Function that determines if an agent gets disrupted.

env Environment in which agents operate.

$fuel\_rate$ Fuel consumption per ton of captured anchovy by a given vessel.

go_fish_t Variable that indicates if a vessel will not fish on a time step t.

$guess\_link$ Function that uses multinomial distribution to connect vessel with producers.

$hours\_day$ Working hours of a plant per day].

$price^p$ Selling price of a given unit of fishmeal.

$price^v$ Selling price of a given unit of landed anchovy.

$prob\_link$ Vector with probabilities of connecting to each producer.

$profit\_rate$ Percentage of the cost that is expected as net profit.

$quota$ Percentage of tac that corresponds to a specific vessel.

$season\_demand$ Demand of fishmeal on a fishing season.

s Supply vector.

tac_vessel Total allowable catch of a given vessel.

tac Total allowable catch.

t Specific time step.

$work_t$ Variable that indicates if an agent will work on a time step t.

$yield\_plants$ Maximum processing yield per day.

$yield\_vessel$ The effective yield of a vessel.

10.1 Introduction

In this chapter, we rely on the use of AFRICA and pacha to develop an operational model of a real case of study. Our motivation is to demonstrate the benefits that an ABM approach, in synchrony with our framework and tool, can provide to the decision making in sustainability studies. More specifically, we aim to enhance the assessment exercise by considering the consequences of disruptive phenomena on a real SN. For this, we selected the Peruvian fishmeal industry as a case study, as it will be described below.

Feed is defined as an edible material used to provide nutrient and energy to an animal diet (FAO, 2001). All feed products, as well as their derivatives (e.g., compound feed), are part of a feed demand that is being simultaneously generated by different industries (e.g., livestock, poultry, aquaculture). For instance, in the aquaculture sector, the most used feed is compound feed resulting from the combination of fishmeal and other vegetable meals (e.g., soybean meal) (Asche et al., 2013; Tacon & Metian, 2015). We focus on this specific feed given the relevance it has in other agricultural supply chains.

The fishmeal production can be described as a reduction process in which fresh anchovy (Engraulis ringens) is transformed into meal through a cooking process, generating fish-oil as coproduct (Fréon et al., 2017).[1] For this chapter, we focus our effort on the fishmeal market, although fish oil may represent an increasing source of revenue for companies.[2] We represent an SN that satisfies a season demand by using three layers: an extraction layer, a production layer, and a demand layer. The production layer contains all actors directly involved in manufacturing, while the extraction layer contains the suppliers with access to natural resources that can have relationships with producer agents (see Fig. 10.1.). Finally, the demand layer encompasses the agents responsable for requesting fishmeal as part of the satisfaction of their own objective (e.g., feed production).

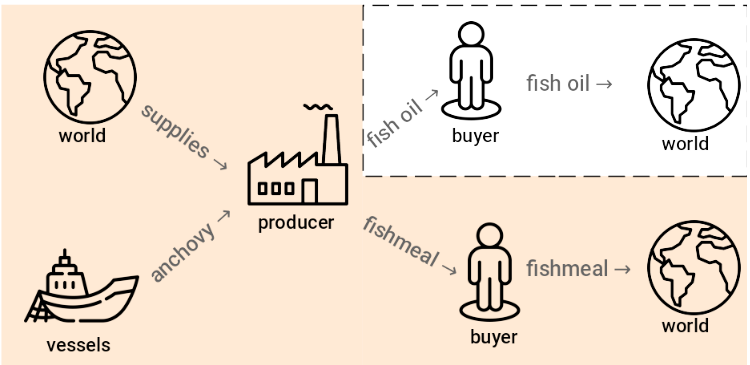


Figure 10.1: Supply network layers. Producers are supplied by the world market and by a vessel fleet. Produced fishmeal is sold to traders that represent the worldwide market. Fish oil is ignored from the model.

There are three main classes of agents: producers, vessel owners, and traders, and an environment as an entity devoid of agency. Producers are responsible for the transformation processes, and they own production plants that operate along the Peruvian coast. A producer is a company that possesses the economic capabilities to sustain non-stop production during a fishing season. In a fishing

[1] Fréon et al., 2017 provides a comprehensive description of the technological system.
[2] This multi-product problem is dealt by performing economic allocation when required.

season, the anchovy is supplied by a fleet of purse-seiner vessels with wooden or steel hull. These vessels can be owned by the production companies or by third party owners that are authorized to only capture anchovy. The availability of this species in the market is set and controlled by the Peruvian Government through the Total Allowable Catch (TAC). This regulation tool is designed to establish capture limits in a period of time (i.e., season) in order to avoid overfishing in open access fishery systems. In this type of system, the output is restricted in order keep the stock biologically safe (Asche & Tveterås, 2004). This TAC is determined for every fishing season, and only authorized vessels can make use of a share of the TAC based on a previously assigned quota (i.e., percentage of the TAC). The individual quota is negotiable and transferable, and in the recent years multiple producers have opted for buying the corresponding share of TAC of other vessel owners in order to increment their own. In this sense, both the TAC and the quota system make the producers' suppliers interact in a closed market.

Peru has played a dominant role in the last 50 years (Asche et al., 2013; Mullon et al., 2009), accounting for at least 18 percent of the worldwide production of fishmeal. Moreover, this industry is one of the most relevant productive activities in Peru, representing around 1.5 percent of the Peruvian Gross Domestic Product (GDP). The production its highly dependent on the supply of anchovy, meaning that it is also exposed to any risk associated with the availability of the resource. Natural risks, such as El Niño South Oscillation (ENSO) phenomenon (Letson & McCullough, 2001; Schreiber et al., 2011), or logistic disruptions (S. Singh et al., 2020) can generate important impacts, for which the industry needs to be resilient. In a similar way, the sustainability of the fish stock (Arias Schreiber, 2012) and the reduction the of Peruvian GHG emissions (Vázquez-Rowe et al., 2019) represent an additional layer of objectives, that, in conjunction with the adequate functioning of the industry, are sustainability targets to achieve.

The study of both environmental sustainability and system's resilience is an ongoing topic of research.[3]. For instance, Berr et al., 2022 proposed a framework to assess these impacts along the supply chain in the short-term and the long-term using an LCA perspective. Disruptions impacts have also been assessed using analytical models of decision in consequential LCA frameworks (de Bortoli & Christoforou, 2020). Nevertheless, as it was discussed in sections 3 and 4.3, our focus is to asses sustainability under a CAS-oriented approach.

While our modelling approach follows a supply system vision, we focus our interest on the fishmeal industry. In this sense, the objective of this chapter is to build an operational ABM model of the Peruvian fishmeal production to understand the consequences that potential disruptions could have on the sustainability of this sector. To accomplish this, we evaluate two types of

[3] See section 3 for wide review of this

disruptions: a medium-term (e.g., ENSO), and a short term (e.g., operational disruptions). For this we propose the study of three scenarios. Scenario A represents the baseline that is modeled using the season 2029-I as reference, while scenarios B and C are focused on medium-term and short-term disruptions, respectively. In section 10.2, we describe the ABM modelling framework components, and the different additional modelling efforts proper to the modelling of socio-technical systems. Finally, we present the results and discussion of our findings in section 10.5.

10.2 modelling methods and network structure

This chapter uses different approaches and toolkits in conjunction to generate an operational model. We start by setting ABM as the main modelling paradigm, which implies adopting a Montecarlo simulation approach (see section 10.2.1.2). During a Montecarlo simulation, multiple models and calculations with their own frameworks and approaches will interact among each other. In order to provide clarity, we represent these interactions and synergies from a methodological perspective in Fig. 10.2. The simulator, built following the pacha framework, is the orchestrator of the different sub-modules that are executed during run-time. For instance, computational agents, modeled using the AFRICA framework, will constantly require to communicate with certain machine learning models. Similarly, when calculating certain impacts or requiring inventory data, agents will appeal to the LCA methodology, which relies on a framework, both theoretically and operationally.

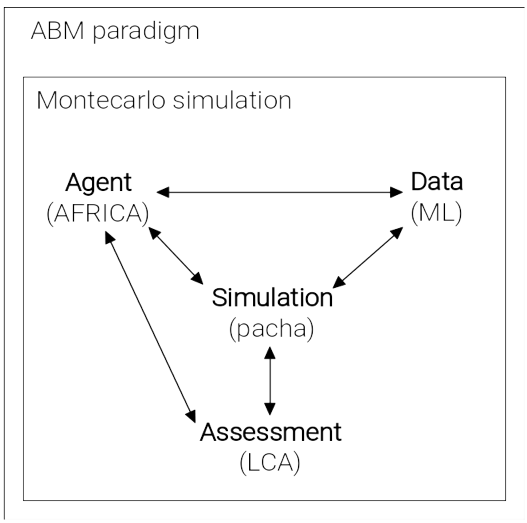


Figure 10.2: Synergies among different frameworks and approaches followed in this chapter. The ABM paradigm includes a Montecarlo simulation approach that, at the same time, encompasses different frameworks and approaches in synergy. ML refers to machine learning and LCA to life cycle assessment

To present the operational blocks of this chapter, we first present a socio-technical model of the fishmeal production using the ABM paradigm (section 10.2.1). We then describe the calculation of the parameters, models, and variables that are inputs of the ABM model (section 10.3).

10.2.1 The ABM model

The main assumption of the ABM model is that the interactions and flows among companies occur to satisfy a given demand $season\_demand$ of fishmeal. For every agent ω, we rely on AFRICA to represent its operational configuration, $\boldsymbol{\theta}$, and on the `pacha.engine.Agent` class to provide an OOP instance that contains the agent's rules programmed as `wake_up` and `run` functions. [4] The operational configuration is a set of arrays describing the relationship among products, processes and factors for an agent (see section 6.3). Both functions of rules and $\boldsymbol{\theta}$ are meant to be programmed as computer code by the practitioner. As defined in section 6, every product flowing in the SN should have at least one supplier agent, whether it is explicitly modeled or assigned to an unconstrained market. The simulation starts with a fixed number of products that are identified after observing every $\boldsymbol{\theta}$. We explicitly modeled heterogeneous vessel owners, fishmeal producers, and fishmeal buyers. The rest of products flowing in the technosphere were assigned to markets that behaved as proxy-agents (see section 10.3.5). In this sense, we define one simulation instance as a set of agents, Ω, and an environment, env, that operate every time step $t \in T$ inside the computational space orchestrated by a `simulator`.[5]

10.2.1.1 Description of the simulation

On the one hand, Ω is defined as the union three sets of agents Ω^v, Ω^p, Ω^b, as representations of the vessel owners, producers, and demand layers, respectively; and the set Ω^m, as the collection of market proxy-agents.[6] Each set contains multiple agents that will not necessarily share the same characteristics but will have similar roles from an SN perspective. Moreover, since agents in a set refer to the same production scheme, we define templates for the operational configuration $\boldsymbol{\theta}$ of each type of agent so they are used as initial states.

On the other hand, the environment env serves as a representation of an omniscient entity with full access to every agent's information, and it is capable

[4] Throughout the manuscript, words presented using this style (`verbatim`) will refer to functions, variables, or artifacts external to the context of this chapter, or that are only used once, so they are not defined with mathematical notation. For instance, `module.function` can refer to a specific function of a module object, and it is not formalized in mathematical notation. Similarly, a mapping function, such as a dictionary that maps parameters to values, can be simply referred as the file that contains the keys and values: `parameters`. In any case, when used, this style will come accompanied by sufficient context.

[5] The `simulator` is an instance of the `pacha.engine.Simulator` class.

[6] In this section, supercripts will refer to a particular subset of a bigger set, or to a specific element of a finite and non-incremental set (i.e., $Variable^{group} \mid group \in a, b$). Meanwhile, subscripts will be used index on a finite sequence (i.e., $Variable_{index} \mid index \in 1, \ldots, 3$).

of modifying any state. In an initial time step $t = 0$, the *env* executes a `setup` function to prepare agents according to the any custom indication. When $t > 0$, *env* executes an `instructions` function, that takes t, Ω, and `parameters.yaml` specifications as inputs to modify agents state if requested.

A simulation of T time steps starts instantiating the `simulator`, and by feeding `run, wake_up, instructions, setup` functions, `parameters.yaml` file and $\boldsymbol{\theta}$ templates.[7] Depending on t, the *env* will start executing `setup` or `instructions` functions. Agents then observe the environment and update their state by executing a `wake_up` function. Afterward, every agent will act one after another in an order provided by a `scheduler`, an instance of the `pacha.engine.Scheduler` class.

The proposed multi-layer structure is not only helpful as a proxy of agents' roles in the network but also to understand the propagation of demand *season_demand* throughout the SN. This demand is initiated by Ω^b, and then transmitted to the producer Ω^p, to finally reach Ω^v. In within layers, agents will execute their `run` function in a random order. ω is reactive, meaning that they can execute actions if requested by other agents (e.g., request for quotation), even when out of turn. Finally, at the end of every time step, the `simulator` will take snapshots of all the states and store then in a structured database (see Algorithm 2).

Algorithm 2: Algorithm followed by the `simu` in for T time steps

Data: Ω = set of all agents, *env* = environment, `instructions` = function that alters states, `setup` = function that alters states, `scheduler` = scheduler object, `Db` = structured database, T = simulation time steps

if $t = 0$ **then**
    env executes `setup`
end
for $t \leftarrow 1$ **to** T **do**
    env executes `instructions`
    for $\omega \in \Omega$ **do**
        ω executes `wake_up` function
    end
    for $\omega \in$ `scheduler`.$order(\Omega)$ **do**
        ω executes `run` function
    end
    $\text{data}_t \leftarrow$ snapshot of all states
    append data_t to `Db`
end

[7] These steps were described in section 7.4

10.2.1.2 Stochastic components and Montecarlo simulation

The proposed ABM is stochastic by nature because it is affected by the stochasticity associated with agents' behaviors, initial conditions and characteristics of the environment. This stochasticity is controlled by random variables, and these, at the same time, are controlled by the initial parameters and seeds. Given the complexity of the model, the expected value of the metrics of interest (e.g., impacts) are determined following a Montecarlo approach.

The designation of random variables responds to the need of presenting the ontological uncertainty of a random phenomenon (e.g., capture rate), or the epistemic uncertainty of unknown or partially known information (e.g., likelihood of going to fish). For these cases, probability distributions can be used to approximate the variance of the random variable. In other cases, probability distributions can be used to speculate or to explore unprecedented events in counterfactuals scenarios. Since our model composed by other models, the simulation follows an error propagation scheme proposed by Paul Baustert, 2021, in which different components of the model are controlled by different random states. In our case, we use two instances of `pacha.tools.RandomGenerators`, one to have independent control the random state of the variables, and other to control the submodels (e.g., LCA databases). For this, multiple simulations, τ should be performed in order to determine the variability of the model. In this sense, the expected value of an impact is estimated as the mean of τ simulations, being τ the number of simulations over which one additional run does not affect the variability of the results (i.e., coefficient of variation).

10.2.1.3 Flows and impacts accounting

`pacha` measures the direct environmental flows of agents, meaning that the SN's impact is the aggregation of each individual impact. Under this logic, adopting a life-cycle perspective would imply modelling the world-wide economy. Since this is not practical, we followed an approach in which we embed the life-cycle flows into the most outer nodes (i.e., market proxy-agents). More precisely, if we consider the world-wide SN as a graph, we can say that our agents compose a dynamic sub-graph, while the rest of nodes compose a static sub-graph. In this sense, the accounting of the SN flows is equivalent to adding the flows of the static subgraph, aggregated in advance (e.g., using LCA), to the flows of the dynamic subgraph that are progressively calculated during run-time. With respect to individual agents, these can only calculate life-cycle flows using the available information. In this sense, every agent will constantly calculate an LCA-based impact for its produced product as the addition of the life-cycle impacts of the supplies and its own direct impacts (see 10.3).

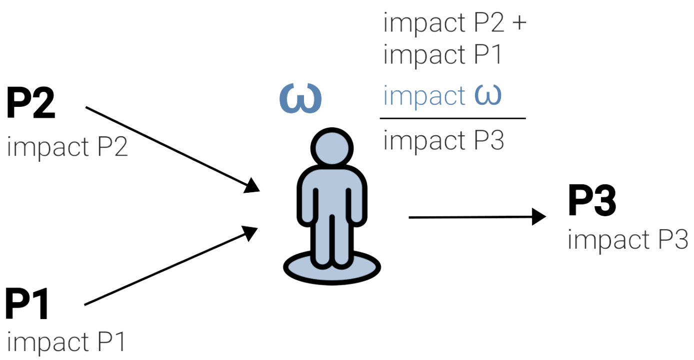


Figure 10.3: Example of the calculation of the life-cycle impact of a product P3 from the perspective of an agent ω. The impact of P3 is the aggregation of the embodied impacts of P2 and P1, and the direct impact of ω.

For this chapter, we used ecoinvent 3.6 (Wernet et al., 2016) as a static supply chain model to obtain the flows of agents in Ω^m. When the dynamic subgraph is a small subset of the full graph, this approach is considerably more efficient than other coupled ABM-LCA implementations because we aggregate the static graph only when required instead of solving for the full technosphere at every time-step [8]. Other implementations of this approach can be found in LCA-related literature, such as (Jolivet et al., 2021) who performed fast LCA calculations of parametric LCA models by aggregating unparameterised background nodes. Nevertheless, it is important to mention two main caveats of this approach. First, the more agents are included in the dynamic graph, the more interactions are required per time step and the more complex the model becomes. Second, nodes that connect the static and dynamic sub-graphs (i.e., market proxy-agents), must have an out-degree and in-degree equal to zero in the static and the dynamic sub-graphs, respectively. This happens because any kind of feedback coming from the dynamic side would modify the static side, which, by consequence, changes the aggregated flows. For efficiency purposes, we converted all biosphere flows into impacts, which were then used into the simulation. Finally, besides the monetary flows, we focused on accounting Global Warming Potential using the IPCC methodology (IPCC, 2006).

10.2.2 Agents and simulation environment

As mentioned before, every agent is controlled by the rules defined in their `run` and `wake_up` functions. At the same time, these depend on the initial conditions set by the variables and parameters fed into the model. This section describes the parametric expressions and algorithms corresponding to each of type of agent. In this sense, just in this section, we avoided the use of the index ω since it was understood from the context.

[8] see C. Davis et al., 2009 for more details of the other ABM-LCA implementation

10.2.2.1 The environment

The main natural resource is the allowed stock of anchovy that is constrained by the TAC, represented by variable *tac*. We assume that *tac* is an exogenous variable since it is determined by policy makers, and controlled by biological and climatic conditions, rather than economic aspects (Asche & Tveterås, 2004; Tveterås, 2002). Nevertheless, only a percentage of these stock, will be transformed to fishmeal, for which we allocated a percentage *allocation* of *tac* to be considered as TAC for modelling.[9]

Agents begin the simulation with their corresponding $\boldsymbol{\theta}$, isolated from each other and without information of other agents' state. For this, the *env* executes its `setup` function to initialize a graph $G(\Omega, E)$, using a set of edges E to connect the agents. This process adds a new purchase process to the decision space for each new connection (see Algorithm 3). The graph $G(\Omega, E)$ will be tripartite since vessels, producers and buyers never connect with agents of the same layer. All producers are connected to all buyers, while connections between vessels and producers are determined by a function *guess_link* (see eq. 10.1). When a vessel $\omega^v \in \Omega^v$ is owned by a producer $\omega^p \in \Omega^p$, *guess_link* adds the edge (ω^v,ω^p) to E. However, when ω^v is independent, function *guess_link* finds a client by sampling from a multinomial distribution, where $n = 1, k = \mid \Omega^p \mid$ and $p = prob\_link$, where *prob_link* is a vector of probabilities to connect to producer. These probabilities were estimated by taking producers' market shares as proxies. The logic is that, in practice, vessels will be more likely to establish a relationship with producers that have a higher share of the market. The function chooses the client whose corresponding position in the sample had a probability of 1, then it adds the edge to E (see eq 10.1).

$$E = guess\_link(\Omega^v, \Omega^p) \cup \{(\omega_a, \omega_b) \mid \omega_a \in \Omega^v \text{ and } \omega_b \in \Omega^b\} \tag{10.1}$$

[9] In following sections, all the different parameters and variables were estimated considering this allocation factor when necessary.

Algorithm 3: Algorithm for the `setup` function of *env* when $t = 0$

Data: E = list of edges, Ω = set of all agents, `parameters.yaml` = parameters file

Function `setup(`Ω, E, `parameters.yaml):`
- **for** $\omega \in \Omega$ **do**
  - update $\boldsymbol{\theta}_\omega$ using `parameters.yaml`
  - **for** $edge \in E$ **do**
    - **if** $\omega \in edge$ **then**
      - connect ω with partner agent
      - add a "purchase process" column to $\boldsymbol{\theta}$
    - **end**
  - **end**
  - perform any custom update of ω
- **end**
- perform any custom update of *env*

On a time step $t > 1$, every agent ω has the freedom to act if its variable $disrupted_t^\omega \in \{0, 1\}$ equals zero, otherwise it will be deactivated from the simulation. The state of this variable is decided every day with a function *disrupt* that is calculated taking all the agents, the time step, and an intensity parameter $disrupt\_rate \in [0, 1]$ (see eq. 10.2). These disruptions are performed in the `instructions` function.

$$disrupted_t^\omega = disrupt(\omega, t, disrupt\_rate) \tag{10.2}$$

$$\tag{10.3}$$

Algorithm 4: Algorithm of `instructions` executed by *env* on a time step t

Data: $disrupted_t^\omega$ = disrupted condition, $disrupt\_rate$ = disruption rate, Ω = set of all agents, t = time step

Function `instructions():`
- **for** $\omega \in \Omega$ **do**
  - $disrupted_t^\omega \leftarrow disrupt(\omega, t, disrupt\_rate)$
- **end**

10.2.2.2 Vessels

On a day t, a vessel owner will decide to fish if a $work_t \in \{0, 1\}$ variable equals 1. This variable is always 1 unless the agent was disrupted or it has a $go\_fish_t \in \{0, 1\}$ value of 0 (see eq. 10.4). Each vessel has a maximum capture capacity equal to $capacity^v$. However, in practice, vessels do not operate at their maximum since their yield is affected by measurable factors, such as available stock in fishing zone or machinery efficiency, and by unmeasurable factors, such as the skipper effect (Joo et al., 2015; Vázquez-Rowe & Tyedmers, 2013). Despite the source of inefficiency, we assume that the maximum daily landed anchovy amount, $yield\_vessel$, will be affected by a $capture\_rate_t \in [0,1]$ factor (see eq. 10.5). With respect to the technological flows, the vessel will have an operational configuration $\boldsymbol{\theta}^v(energy)$ parameterised by an energy consumption factor $energy$. Finally, the $energy$ represents the average net energy (MJ) spent in the fishing effort, this is calculated using a $fuel\_rate$ factor, which indicates the consumption in gallons of diesel per ton of landed anchovy (see eq. 10.6).

$$work_t = \begin{cases} 0, \text{if } go\_fish_t = 0 \text{ or } disrupted_t = 1, \\ 1, \text{if otherwise} \end{cases} \tag{10.4}$$

$$yield\_vessel_t = capacity^v \times capture\_rate_t \tag{10.5}$$

$$energy = fuel\_rate \times 146.52 \frac{MJ}{Gal} \tag{10.6}$$

In a season, a vessel will try to fish at its maximum $yield\_vessel$ until exhausting its maximum allowed catch tac_vessel. This value is a percentage $quota$ of tac, permanently assigned to this specific vessel (see eq. 10.7). In this sense, the decision of starting a day follows the logic presented in algorithm 5. If $work = 1$, vessels will have to solve an instance of the sourcing problem ϕ to determine the supply vector $\boldsymbol{s}$ that allows to produce tac_vessel (see eq. 10.9).[10] Using the AFRICA framework, $\boldsymbol{s}$ and $\boldsymbol{\theta}$ will then be used to make requests to the suppliers (i.e., markets in Ω^m), transform inputs into anchovy, and calculate the unitary cost, $cost^v$.[11] The selling price, $price^v$, will be set by increasing $cost^v$ by a factor $profit\_rate \in \mathcal{R}^+$, as shown in eq. 10.8 The agent will finally account for its direct impacts and the life-cycle impacts of the anchovy by using the information received from their suppliers following the logic explained in Fig. 10.3 (see algorithm 6).

$$tac\_vessel = tac \times quota \tag{10.7}$$

$$price^v = cost^v \times (1 + profit\_rate) \tag{10.8}$$

$$\boldsymbol{s} = \phi(yield\_vessel_t; \boldsymbol{\theta}) \tag{10.9}$$

[10] eq. 10.9 was previously presented in section 6.3 as eq. 6.2 that considered a vector $\boldsymbol{y}$ as parameter. While we show that eq. 10.9 uses a scalar, it is assumed that it will be reshaped into a vector to be operated.

[11] This has been explained in section 6.3.5 and its handled by the `pacha.engine.africa` module that has the computational implementation of the AFRICA framework.

Algorithm 5: Algorithm of `wake_up` function of a vessel agent

Data: $disrupted$ = disrupted condition, go_fish = go to fish condition, $yield\_vessel_t$ = maximum landed anchovy in a time step, tac_vessel = maximum allowed catch for a vessel, $work$ = go to work condition

Function `wake_up()`:
- $work \leftarrow 1$
- **if** $disrupted = 1$ *or* $go\_fish_t = 0$ **then**
  - $work \leftarrow 0$
- **end**
- $total\_catch \leftarrow$ sum$yield_vessel_t$ from 0 to t
- **if** $total\_catch \geq tac\_vessel$ **then**
  - $work \leftarrow 0$
- **end**

Algorithm 6: Algorithm of `run` function of a vessel agent in time t

Data: ϕ = function of production, $yield\_vessel_t$ = maximum landed anchovy in a time step, $\boldsymbol{\theta}$ = operational configuration, $\boldsymbol{s}$ = supply vector, $work$ = go to work condition

Function `run()`:
- **if** $work = 1$ **then**
  - $\boldsymbol{s} \leftarrow \phi(yield\_vessel_t; \boldsymbol{\theta})$
  - make requests for purchase as indicated in $\boldsymbol{s}$
  - transform inputs and store the outputs
  - $cost^v \leftarrow$ using$\boldsymbol{s}$
  - calculate $price^v$ using $cost^v$
  - calculate direct and life-cycle impacts
- **end**

10.2.2.3 Producers

Fishmeal producers represent the intermediates of the demand flow since they are the link between the resource extraction side and the consumption side. These agents operate at their maximum processing capacity $capacity^p$ (i.e., Tn/hr) during $hours\_day$ hours a day, leading to a maximum processing yield $yield\_plant$ (see eq. 10.10). Similar to other small pelagic fisheries, the anchovy fishery and fishmeal industries can be represented as oligopolistic systems where two main commodities are negotiated (Mullon et al., 2009). In this sense, we consider that producers are price takers meaning that they do not have influence on the overall supply of anchovy and their will equal their selling price, $price^p$, to the current market price. Finally, `wake_up` and `run` functions can be described in algorithms 8 and 7, respectively.

$$yield\_plant = capacity^p \times hours\_day \tag{10.10}$$

Algorithm 7: Algorithm of `wake_up` function of a fishmeal producer agent

Data: $disrupted$ = disrupted condition, $yield\_plant$ = maximum fishmeal production in a time step, $work$ = go to work condition

Function `wake_up()`:
    $work \leftarrow 1$
    if $disrupted = 1$ **then**
        $work \leftarrow 0$
    end

Algorithm 8: Algorithm of `run` function of a fishmeal producer agent

Data: ϕ = function of production, $yield\_plant$ = maximum fishmeal production in a time step, $\boldsymbol{\theta}$ = operational configuration, $\boldsymbol{s}$ = supply vector, $work$ = go to work condition

Function `run()`:
    if $work = 1$ **then**
        $\boldsymbol{s} \leftarrow \phi(yield\_plant; \boldsymbol{\theta})$
        make requests for purchase as indicated in $\boldsymbol{s}$
        transform inputs and store the outputs
        $cost^p \leftarrow using\boldsymbol{s}$
        $price^p \leftarrow marketprice$
        calculate direct and life-cycle impacts
    end

10.2.2.4 Buyers

We considered market prices, $price^b$, and season demand, $season\_demand$, as exogenous variables. Each buyer agent represents the aggregation of the demand of a specific country, $buyer\_demand$, which is a percentage $demand\_share$ of the $season\_demand$ (see eq. 10.11). We assume that this demand will be requested on a daily basis, $daily\_demand$, following a constant fashion (see eq. 10.12) Finally, `run` function can be described in algorithms 9, while `wake_up` is ignored since it is trivial (i.e., $work = 1$).

$$buyer\_demand = season\_demand \times demand\_share \tag{10.11}$$

$$daily\_demand = \frac{buyer\_demand}{T} \tag{10.12}$$

Algorithm 9: Algorithm of `run` function of a fishmeal buyer agent

Data: ϕ = function of production, $daily\_demand$ = demanded quantity in a time step, $\boldsymbol{\theta}$ = operational configuration, $\boldsymbol{s}$ = supply vector, $work$ = go to work condition

Function `run()`**:**
- **if** $work = 1$ **then**
  - $\boldsymbol{s} \leftarrow \phi(daily\_demand; \boldsymbol{\theta})$
  - make requests for purchase as indicated in $\boldsymbol{s}$
  - transform inputs and store the outputs
  - calculate direct and life-cycle impacts
- **end**

10.3 Model inputs and data analysis

We feed the model with both qualitative and quantitative data that were obtained from public sources, surveys, proprietary databases, and personal communication with stakeholders. We selected the first fishing season of the year 2019 as a reference since it represent the year with more available data. The parameter values, models, and initial conditions were determined from the analysis of the available information. In this section, we describe the rational and the different steps that we followed to obtain these parameters and models.

10.3.1 Anchovy fishing fleet: a stochastic model

The simulation environment takes as input a set of heterogeneous agents that will perform the fishing activity in a simulation run. While the current fishing fleet could be explicitly described in terms of the vessels and their properties, we argue that a deterministic representation of this fleet would describe a specific state, but not its full properties. Due to that our objective is to model multiple states of the fleet, we decided to use a synthetic fleet model to have an infinite source of fleet states. The synthetic fleet model is a statistical model, $P(X)$, of the joint probability distribution of the vessels characteristics, being $X = (X_1, \ldots, X_n)$ the random vector of n random variables. The model can be used to sample new instances of data (i.e., synthetic fleets) that follow the same statistical properties of the real fleet. In practice, the benefits of relying on a synthetic population fleet model are twofold. First, since the model is stochastic, it provides a convenient way of introducing correlated samples for the Montecarlo simulations. This occurs because the different parameters are sampled from a joint probability distribution, instead of assuming independence as it is commonly done in other LCA approaches (Groen et al., 2014; Lloyd & Ries, 2007). Second, the anonymity of the vessels names and their owners can be guaranteed.

Table 10.1: Peruvian anchovy fishing fleet - statistics

	Length (m)	Power	Capacity (Tn)	TAC (%)
mean	26.07	537.17	197.70	0.13
std	12.16	452.35	176.50	0.13
min	11.23	0.00	0.00	0.01
25%	15.80	238.62	61.83	0.03
50%	21.13	402.67	108.80	0.06
75%	36.60	634.00	333.32	0.20
max	77.00	3951.00	1108.10	0.84

The use of predictive approaches for inventory building has been previously applied in studies related anchovy fishing. For instance, A. Avadí et al., 2014 used a linear regression to predict the tonnage of the complete fleet when building the life-cycle inventory. However, at the best of our knowledge, no uncertainty-related treatment has been conducted in studies of this industry. In this sense, the construction of the generative model consisted in two stages: a stage of data analysis and feature engineering, and a stage of proper training of the generative model.

To understand the characteristics of the Peruvian anchovy fishing fleet, we relied on two main sources of information. Firstly, we used the national registry of fishing vessels as the main reference of ships characteristics (PRODUCE, 2023a). The database contains detailed information of all the 750 ships regarding ownership, size, weight, power, type of hull, and individual tac_vessel. This tac_vessel is a percentage that corresponds to the allowed share of tac and it has been previously set by the Peruvian authorities based on the $capacity^v$ and yearly performance (see Table 10.1). Secondly, we relied on a database consisting on primary company data that contains information about ships performance. This data depicts monthly fuel consumption and yield that were gathered at the moment of landing.

The fleet is heterogeneous in terms of physical characteristics, but also with respect to the participation of each individual vessel in the activity. As shown in Fig. B.1a, most of the vessels have an individual TAC inferior to 0.1 percent. From this group, the majority, also known as vikings, have a wooden hull. However, despite the abundance of wooden ships, almost 80 percent of the total quota has been allocated to steel vessels (see Fig. B.1b).

The distinction between steel and wooden hull is relevant also from a non-physical perspective. Information regarding regulation compliance of wooden hull vessels is more scarce, differently from the steel vessels that are more regulated. This implies that the interactions among wooden hull vessel owners regarding some social aspects (e.g., pensions, benefits) may obey some particular dynamics that do not follow the conventional practices (e.g., illegal or irregular activities). Nevertheless, given the absence of information, we consider that the activities of both types of vessels responds to the norms and regulations of the country.

From a production perspective, this heterogeneity is important since diesel consumption and fishing patterns can depend on ship's characteristics. In this sense, we expressed diesel consumption in terms of its use per ton of landed anchovy (i.e., gallons/ton), which can be understood as a proxy of the effective fishing effort. This simplification allows us to reduce the algorithmic complexity of the simulations since the marine logistics of the fishing activities are aggregated into one consumption factor. The rate is calculated by dividing the total monthly consumption of diesel by the total tons of landed anchovy. Unfortunately, this database contained sensitive data only for a group of 214 vessels, meaning that there were still 536 ships without that information. As it is shown in Fig. 10.4, $fuel\_rate$ is correlated to some properties of the fleet, meaning that it is feasible to propose a function to map vessels characteristic to $fuel\_rate$. In this sense, we proposed a machine learning model that can be used as a mapping function in order to perform predictions for the rest of the fleet.

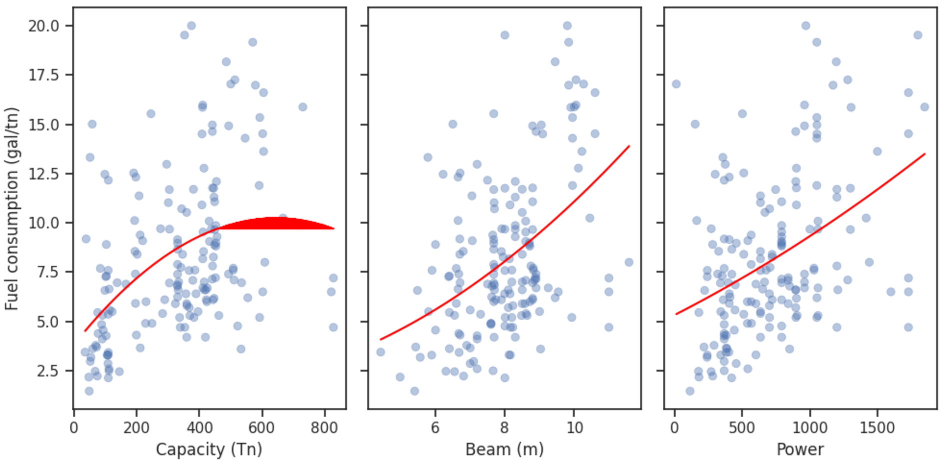


Figure 10.4: Correlation between fuel consumption rate, and three vessel's characteristics. fuel consumption rate is expressed in gallons of diesel consumed per ton of landed anchovy. Red line shows the best fit to a polynomial curve of second order. Variables like Power and Beam indicate monotonic correlation, while Capacity shows a non-monotonic correlation.

For this purpose, we selected an XGBoost algorithm (Chen & Guestrin, 2016) to train a model that takes six continuous and three categorical input variables to predict *fuel_rate* (see Table 10.2). The categorical variable *buyer* represents the group to which the vessel owner supplies. These groups correspond to the fishmeal plants that can be potential buyers at a given fishing season. In some cases, the fishmeal plant agent also owns vessels, meaning that the vessel-buyer connect is already assigned. When more than one company can be a potential client, the category label will be a concatenation of these clients using a separator (i.e., ';'). In the case of the absence of a potential buyer, a label 'None' determined the flexibility of the vessel to supply to any fishmeal producer. The training data was split in two sets of 30 and 70 percent for training and validation, respectively. We used a randomized search method to identify the best hyperparameters that minimized the selected performance indicator (i.e., coefficient of determination R^2).

Table 10.2: Variables used in the XGBoost model that predicts *fuel_rate*

Variable	Mean	Domain
Length	34.0	12.0 - 77.0
Beam	8.0	4.0 - 13.0
Depth	4.0	1.0 - 8.0
Capacity (Tn)	317.0	35.0 - 1108.0
Power	741.0	10.0 - 3951.0
Capacity (M3)	311.0	34.0 - 1080.0
Material	-	[wooden, steel]
Refrigeration	-	RSW, ICE, None
buyer	-	[<buyers/owners>]
fuel_rate	9.0	1.0 - 38.0

For the generative model we selected a Gaussian Copula model (Patki et al., 2016). A Gaussian copula is a joint probability distribution function based on the Sklar's theorem that states that all multivariate distribution functions can be represented by a combination of the marginals and a copula containing the dependencies among variables. A copula is a multivariate distribution function with marginals uniformly distributed in the range of $(0, 1)$ (Durante & Sempi, 2010). In the Gaussian copula $\mathcal{C}_\Sigma$, the function is a standard multivariate normal distribution, Φ_Σ, with mean zero and with the same covariance matrix Σ as of the random vector X. When marginal distributions $F_1, ..., F_n$ are known, a random vector $\mathbf{X} = (X_1, ..., X_n)$ can be generated by sampling values from the copula to then plug them into F^{-1}, as depicted in eq. 10.13.

$$\mathcal{C}_\Sigma(\mathbf{X}) = \Phi_\Sigma(\Phi^{-1}(F_1(X_1)), \dots, \Phi^{-1}(F_1(X_n))) \tag{10.13}$$

10.3.2 Vessel landings

The season 2029-I started on April 29th, and finished on July 31st with an authorized $tac = 2.013 \times 10^6$ tons, setting the main constraint of the fishing labor. In this sense, to understand the patterns of fishing activity, we observed all the landings for each type of vessel in the season 2029-I. Vessel owners unload the fresh anchovy directly at the fishmeal producer's port. The landed quantities are commonly gathered by the producers themselves in ports along the Peruvian coast and verified by the national authorities. We built our database by collecting daily the landing logs registered by the Peruvian Sea Institute (IMARPE, 2021). We observed that two main ports (i.e., Chimbote and Chicama) group the majority of the landings in a constant fashion, while the rest of ports reach a plateau at the mid of the season (see Fig. B.3).

When observing the numbers of vessels that land fish every day, we note that wooden vessels are abundant at the beginning, and scarce by the mid of season, while the number of steel vessels only decreases by the end of the season (see Fig. 10.5). If we observe the daily landings, we note that for wooden vessels this decrease matches a high value of consumed TAC. From this, one could speculate that this aggregated behavior results from wooden vessels exhausting their individual TAC by the mid of the season (see Fig. 10.6).

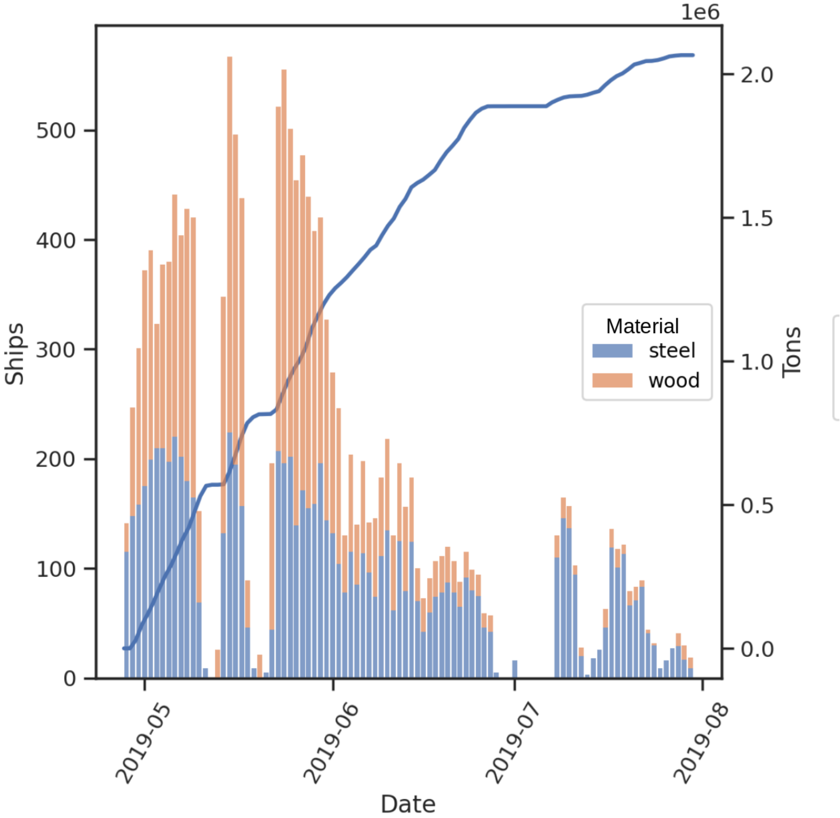


Figure 10.5: Numbers of landings per type of vessel (bars and left axes) and accumulation of landed anchovy (blue line and right axes) for the fishing season 2029-I.

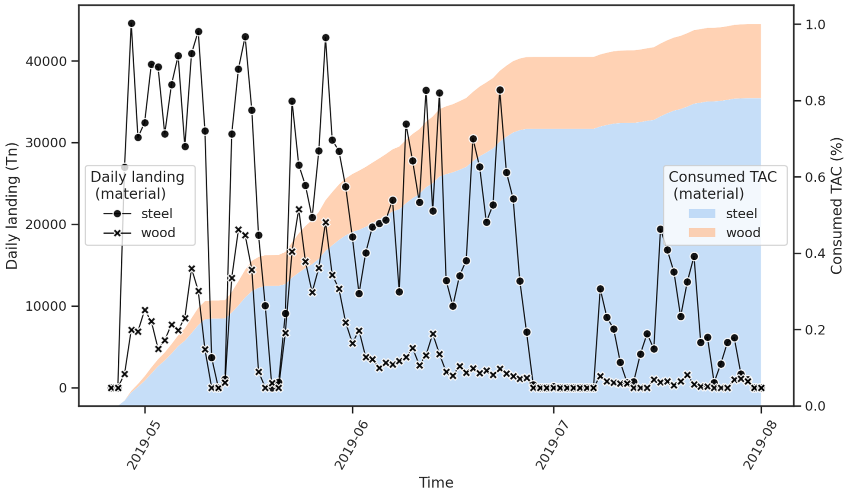


Figure 10.6: Daily landings (lines and left axes) and cumulative consumed TAC (colors and right axes) per type of vessel in the fishing season 2029-I. It is shown that wooden vessels exhaust their individual TAC by the mid of the season.

While we are capable of modelling the seasonal trend by assigning an individual tac_vessel for each vessel agent, we are not capable of explaining the daily variability among vessels or the variability among days (i.e., from one day to another). This was the initial motivation to define the defined a go_fish_t variable. The rationale behind the use of this variable is that, besides the known behaviors and constraints, there is still an unknown component that influences the final decision. We model the fishing decision as a Bernoulli trial parametrized by a $fishing\_prob_t$ parameter. Every time step t, a realisation of the Bernoulli sampling will assign a value for the fishing decision go_fish_t (i.e., 0 or 1). Due to lack of yearly data, we estimated $fishing\_prob_t$ as the percentage of vessels of each type that fished on a specific day t during the 2029-I season.

10.3.3 Individual capture rate

To understand the characteristics of the $capture\_rate$ variable, we relied on a database of daily landings of the season 2021-1 provided by the biggest fishmeal producer in the country (personal communication). Differently from the previous dataset, this database contained detailed measures of departure, arrival, and waiting times, and total capture for each vessel of the company (i.e. steel) and for each vessel of the third party suppliers (i.e., wooden). By dividing the quantity of landed anchovy by the vessel capacity, we determined the real individual capture rate on a daily basis. As it can be observed in Fig. 10.7, wooden vessels have, in average, a higher capture rate that remains higher than the steel vessels' capture rate most of the season. In a season period, the capture rate decreases for all the vessels, regardless of their type (see Fig. 10.7) or their maximum capacity (10.8).

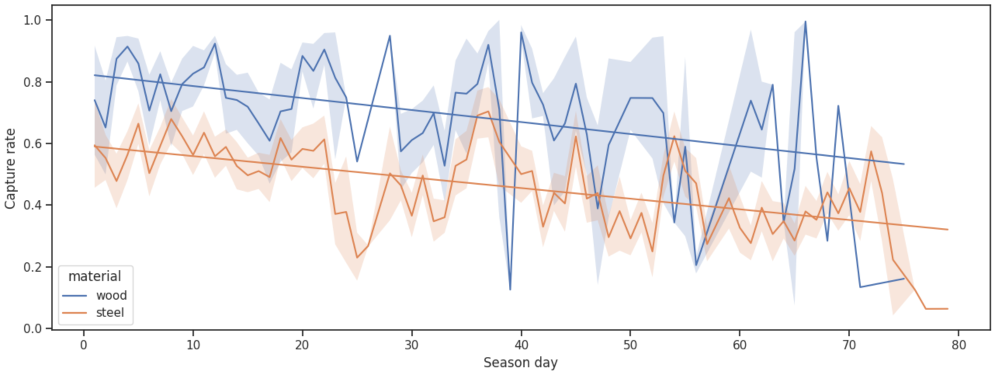


Figure 10.7: Capture rate (landed/capacity) variation for the 2021-1 season for each type of vessel

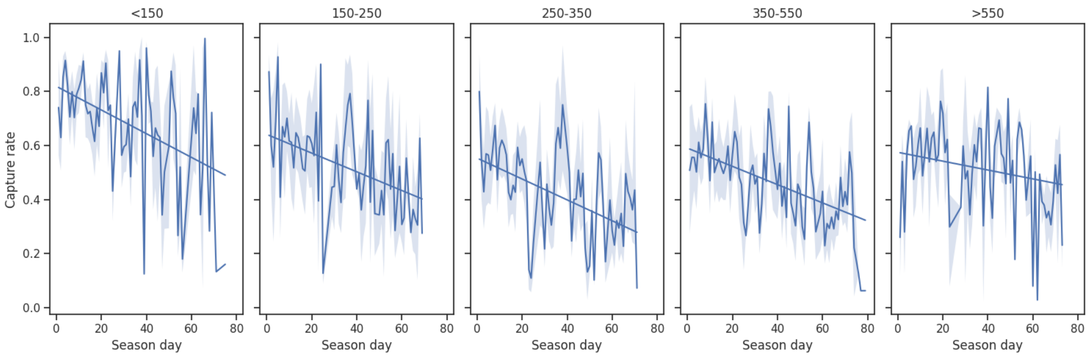


Figure 10.8: Capture rate (landed/capacity) variation for the 2021-1 season grouped by maximum capacity

As it was shown, the capture rate varies over time and depending on the type of vessel. In this sense, to include this phenomenon in the ABM, it was necessary to represent the temporal variability as well as the variability among vessels on daily basis. To this aim, we proposed a function capable of mapping the day of the season, t, and the vessel type to a probability distribution using a gaussian process model. A gaussian process is a stochastic process that can be understood as a collection of random variables indexed by time (Görtler et al., 2019). When used for regression, the model combines normal multivariate prior and updates it using the training data. The prior's covariance is shaped by previously defined kernels, and the kernel hyperparameters are updated during training. In practice, the prediction on a given day t will be a normal distribution parametrized by a mean μ_t and a standard deviation σ_t. In other words, we use the gaussian process as a regressor $\mathcal{GP}$ expressed in eq. 10.14. Finally, the adequacy of the regressor was measured using the coefficient of determination, R^2, as indicator.

$$\mathcal{GP}(t) = (\mu_t, \sigma_t) \tag{10.14}$$

The distributions predicted by $\mathcal{GP}$ have a domain in the range of $(-\infty, \infty)$. This would not be suitable because our probability must be in the range of $[0, 1]$. To overcome this, we represent the normal distribution as a beta distribution with parameters α_t and β_t described by eqs. 10.15 and 10.16, respectively. The new beta distribution will have the same mean and variance of the sampled normal distribution with a domain in $[0, 1]$ (Cribari-Neto & Zeileis, 2010). Finally, the capture rate parameter, $capture\_rate_t$ hereafter, will follow a beta distribution, as shown in eq. 10.17.

$$\alpha_t = \left(\frac{1-\mu_t}{\sigma_t^2} - \frac{1}{\mu_t}\right)\mu_t^2 \tag{10.15}$$

$$\beta_t = \alpha_t\left(\frac{1}{\mu_t} - 1\right) \tag{10.16}$$

$$capture\_rate_t \sim \text{Beta}\left(\alpha_t,\ \beta_t\right) \tag{10.17}$$

10.3.4 Fishmeal processing rate and market data

We relied on public and proprietary databases to identify the companies and to derive relevant variables and parameters. First, we consulted the national fishing plants database (PRODUCE, 2023b). This source contains information about the processing capacity (i.e., $capacity^p$) of 728 authorized industrial and artisanal plants in the country. Moreover, source also included data about ownership, location, and type of activity. We assumed that plants operated 24 hrs per day during a fishing season (i.e., $hours\_day = 24$). From this, we selected only active fishmeal producing plants, filtering out those producing residual fishmeal. [12] The filtering resulted in a set of 89 fishmeal plants that were then aggregated by the company name.

To identify the exports, we relied on the Veritrade database that aggregates all the country daily imports and exports in terms of quantity (i.e., Tons), price (i.e., FOB price), and destination (Veritrade, 2023). We analyzed the exports of the 2017-2021 period to identify the agents exposed to the world fishmeal market. We found that in this period 79 different companies exported to different countries. Nevertheless, only a group of 13 possessed 95 percent of market share, and only 10 of them were part of the group consistently during these five years

[12]Residual fishmeal is low quality type of fishmeal produced with residues of other fishing supply chains and demanded mostly in the domestic market.

(see red line in Fig. 10.9). In this sense, we selected these 10 companies as the fishmeal producers to be modelled as producer agents and we used their corresponding market shares as *prob_link* vector. It is important to mention that a company was modeled as the aggregation of the processing capacity of all of its plants, and the initial price of the model is the one obtained from the average market data (see Table 10.3) .[13]

[13]This simplification was conveniently done to avoid the algorithmic complexity that modelling logistics imply.

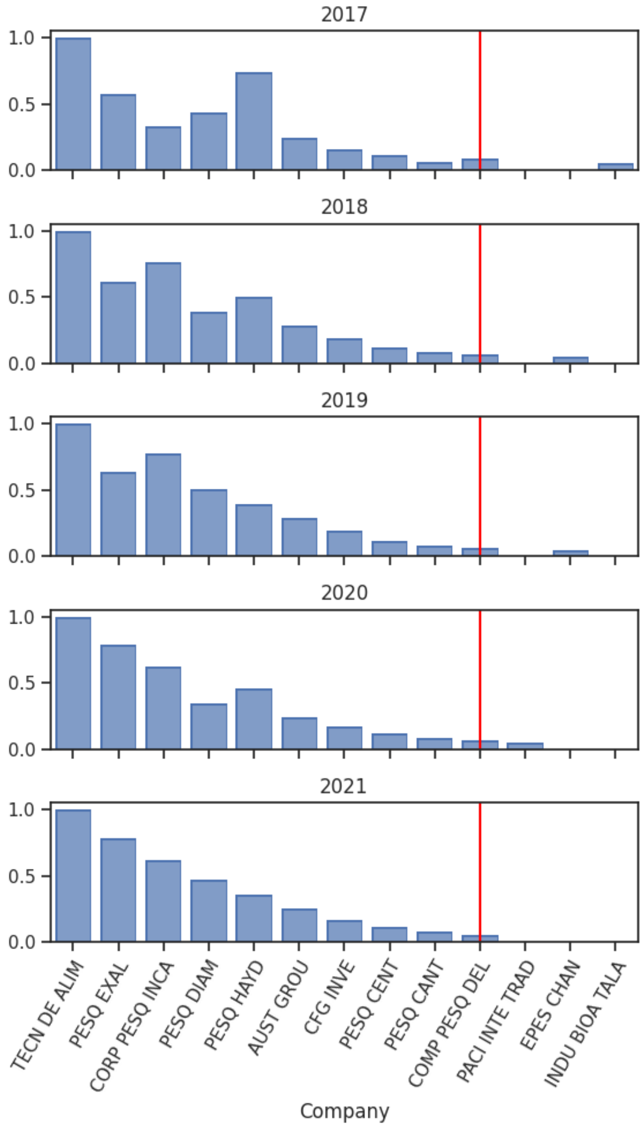


Figure 10.9: Companies that possess 95 percent of the fishmeal market share for the period 2017-2021. Red line separates companies that belonged to this group consistently.

Table 10.3: Fishmeal companies considered in the model

Company	Price (USD/Tn)	Market share	Processing capacity (Tn/Hr)
TECN DE ALIM	1488.32	0.22	1524.00
CORP PESQ INCA	1399.30	0.14	837.00
PESQ EXAL	1434.09	0.13	604.00
PESQ DIAM	1430.90	0.11	964.00
PESQ HAYD	1423.58	0.10	749.90
AUST GROU	1437.07	0.09	593.00
CFG INVE	1427.03	0.08	615.00
PESQ CENT	1458.12	0.04	245.00
PESQ CANT	1409.42	0.02	106.00
COMP PESQ DEL	1444.81	0.01	336.00

With respect to anchovy prices, we consider that local producers are price takers, and they do not have influence on the overall supply of anchovy. In this sense, vessels will always look to exhaust their *tac_vessel* and sell much as possible. Following the same logic, we set the price of a ton of anchovy to USD 200, when bought from a third party, and USD 100 when captured with own vessels (personal communications, 2021). With respect to the fishmeal prices, although the Veritrade database contained information about specific buyers, we desisted of using it because it was incomplete for a several group of exports. Instead, we modeled a trader for each country that imposes fixed daily demand to the producers. Evidently, this is a simplification because the negotiation and delivery processes follow jointly a non linear pattern.[14]

In a logic similar to the selection of producers, we observed the patterns of exports for the period 2017-2021, an we selected the countries that represented the 92 percent of the exports. For this, we calculated the average and the standard deviation of the price paid to the producer companies in the year 2019 (see Table 10.4). The *season_demand* was the sum of all exports, *demand_share* and *price_b* were obtained from the observed shares in season 2029-I (see Table 10.4).[15]

[14]As shown in Fig. B.7, the delivery of products is delayed some weeks from the start of the season.

[15]The demand shares showed a consistent behavior during years 2017-2021. Therefore, it could be assumed that changes in these proportions are highly unlikey.

Table 10.4: Countries with more than 92% of demand share - Season 2029-I

Destination	Exported (MM Tn)	Revenue (MM USD)	*demand_share*	*price*[b] (USD / Tn) - mean
JAPAN	0.07	110.20	0.07	1450.76
ECUADOR	0.01	9.66	0.01	1471.44
TAIWAN	0.02	36.13	0.02	1454.95
CHINA	0.78	1118.50	0.74	1434.07
CHILE	0.02	24.16	0.02	1442.47
GERMANY	0.03	45.66	0.03	1554.94
VIETNAM	0.04	60.37	0.04	1402.04

10.3.5 Operational configuration

For every type of agent, a template of an operational configuration was generated, and it consisted in a collection of arrays that followed the AFRICA framework.[16] Each template depicted an operational configuration with production and storage selection processes that are meant to be updated later during the simulation (i.e., values and dimensions). Proxy-market agents were obtained from the ecoinvent 3.6 database (Wernet et al., 2016). We relied on the life cycle inventories for wooden and steel vessels supplied by Á. Avadí et al., 2014; Fréon et al., 2014, which we parametrised with the values obtained from our models (see Fig. 10.10).

Decision matrix $\boldsymbol{A}$	landed anchovy, fresh	diesel, burned in fishing vessel PE	purse seiner, steel	purse seiner maintenance, steel	lubricating oil	diesel	Storage selection processes
landed anchovy, fresh	1	0	0	0	0	0	
diesel, burned in fishing vessel PE	*energy_cons*	1	0	0	0	0	
purse seiner, steel	-1.9E-09	0	0	0	0	0	$\boldsymbol{I}_{6x6}$
purse seiner maintenance, steel	-1.9E-09	0	0	0	0	0	
lubricating oil	-8.1E-05	0	0	0	0	0	
diesel	0	-0.02	0	0	0	0	

Figure 10.10: Parametrised decision matrix of a steel vessel agent. *energy* variable is meant to be updated for every Montecarlo simulation

With respect to the production plants, we adapted the fishmeal production inventories elaborated by Fréon et al., 2017, in which we split and aggregated nodes in order to distinguish the boundaries of action. A simplified graphical representation of the reference technosphere can be observed in Fig. 10.11, which shows the different activities producing the products required by a fishmeal producer. As it was described in section 10.2.1, certain values in the operational configuration will be modified during run time due to the information flow. Finally, we set the *allocation* parameter as 0.7, which corresponded to an approximation of the economic allocation performed in ecoinvent. This was required since background life cycle inventories were available for by-products and not the joint fishmeal and fish oil production.

[16]These templates are available as excel files in section 13.

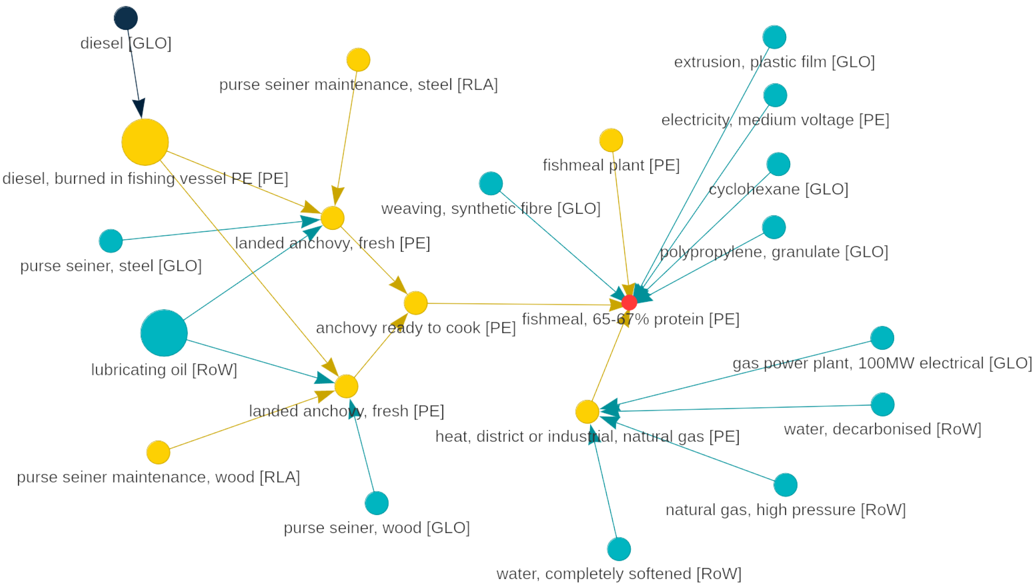


Figure 10.11: Simplified visualisation of an LCA model of the operational technosphere surrounding a fishmeal producer (red node). Teal and yellow nodes represent market activities and transformation activities respectively.

10.4 Modeled scenarios

10.4.1 Scenario A: baseline

The baseline scenario consisted in the simulation of the production of year 2029-I under business-as-usual conditions. In this scenario, no disruptions where introduced, and it was used as a validation and verification benchmark. For this purpose, we selected "landed anchovy accumulation" and the "average life-cycle impact of a kilogram of fishmeal" were selected as validation metrics. The $season\_demand = 4.7e5$ corresponded to tons of exports in the period between July 28th and November 13th. We used the real fleet combined with all the parameters described in the previous section with the mere purpose of validating the machine learning models. Finally, a $\tau = 60$ was used for all the Montecarlo simulations after assessing the convergence of the coefficient of variation (see Fig. B.8).

10.4.2 Scenario B: medium-term disruptions

This scenario attempts to recreate important variations on the supply of anchovy with a medium-term perspective. The principle is that the affectation on the system is inter-seasonal, so it can be represented as a change of some initial conditions of env. For instance, this can be the case of the ENSO phenomenon, which reduces the availability of anchovy in the whole Peruvian sea, affecting equally to all the vessel owners of the system. To simulate this effect, we multiply vessels $capture\_rate$ by an artificial $decrease \in [0,1]$ variable that will reduce the capture capacity of every vessel. This reduction is performed by env at the beginning of the simulation, for which we considered different $decrease$ values, being 1 equivalent to no affectation, and being 0 a complete reduction of the $capture\_rate$.

10.4.3 Scenario C: short-term disruptions

In this scenario, we tried to understand the changes on the system due to unforeseen and unexpected disruptions. The keystone of this scenario is that the effect is sudden and localised on an specific component of the network (i.e., operational disruption). For example, accidents, strikes, attacks, or the simple unexpected shortage of a supply can restrict the normal functioning of vessels, that will consequently affect the fishmeal production. To simulate this effect, we program env to deliberately deactivate vessels nodes on a daily basis in two periods of time. In a simulation of $T = 90$ days, the disruptions occur when $t < 30$, encompassing the period of higher activity, or when $t > 30$, encompassing a longer but less active period of the fishing season. We set these arbitrary ranges to have a window of observations to be able to distinguish agents' operations under normal and disrupted conditions. The $disrupted$ function (presented in eq. 10.2) samples a percentage $disrupt\_rate \in [0,1]$ of agents from Ω^v, all with the same probability of being selected without repetition. We simulated different values of $disrupt\_rate$, where being closer to one means a higher percentage of disrupted agents.

10.5 Results and discussion

10.5.1 Generative fleet model

Since the generative model relies on two submodules, we validated first the performance of the $fuel\_rate$ predictive model. After multiple iterations and tuning (i.e., >9000 iterations), we opted for a regressor with 189 trees. When evaluating on the training and validations set, a performance of $R^2 = 0.78$ was obtained. This can be visually depicted in Fig. 10.12. With the model trained, a predicted fuel_predict value was assigned to each one of the remaining vessels of the real vessels database.

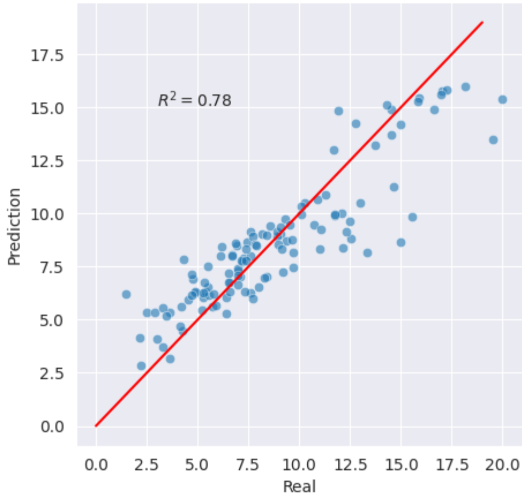


Figure 10.12: Scatterplot of real (x axis) and predict (y axis) fuel consumption rate values using the training and validation sets. XGBoost regressor with 189 trees

In a similar way, different marginal distributions were evaluated when fitting the Gaussian copula model. Once defined, we verified the distribution of the synthetic data by sampling a set of 750 vessels and comparing their statistics with the real fleet database. When it respects to the categorical variables, the model can generate a synthetic fleet with similar wooden/steel ratio and refrigeration systems (see Fig. 10.13).

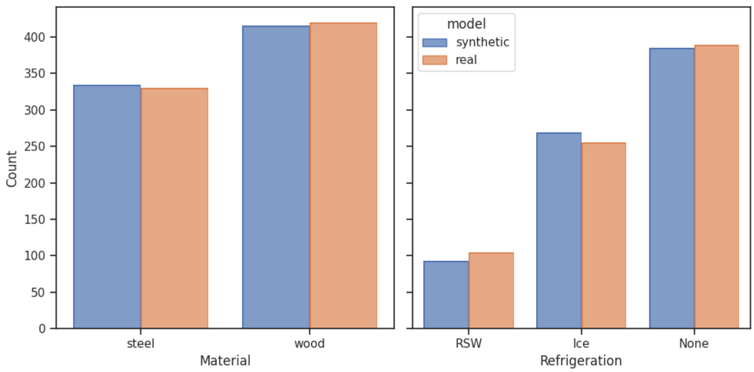


Figure 10.13: Counts of types of synthetic vessels in a sample of 750 in comparison with the real database (i.e,. 750 vessels)

Regarding the numeric data, we also verified that variables, such as capacity, power, TAC, and fuel_fish, show the same marginal distributions as the ones shown in the real data (see Fig. 10.14). Moreover, when comparing the joint distributions, we observe that the generative model can generative samples with the same correlations as the real data (see Fig. 10.15) Finally, when it respects to the distribution of potential buyers, Fig. 10.16 shows that the proportion of vessels corresponding to each type of buyer is similar to real proportion.

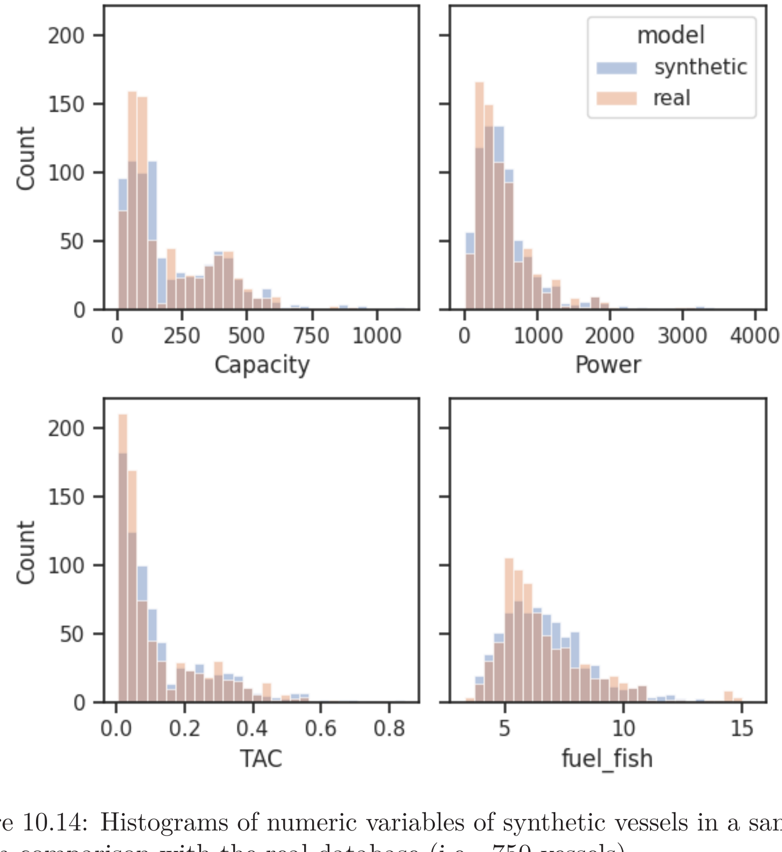


Figure 10.14: Histograms of numeric variables of synthetic vessels in a sample of 750 in comparison with the real database (i.e,. 750 vessels).

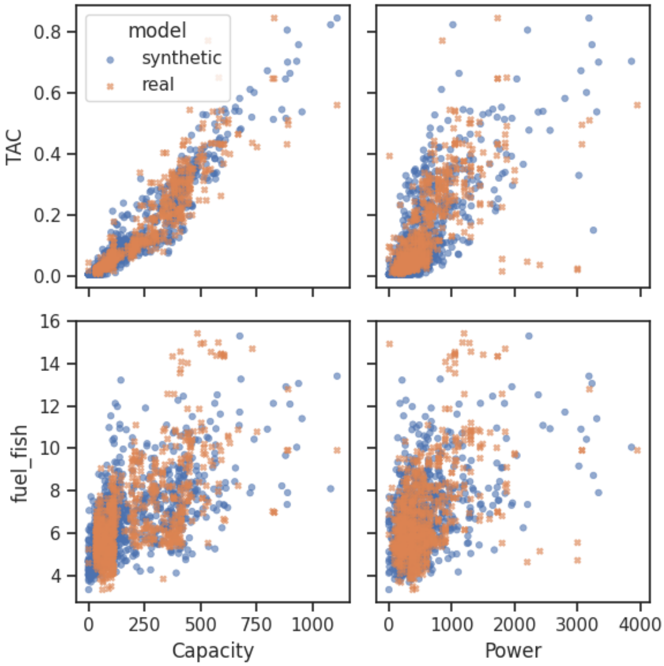


Figure 10.15: Scatterplot of distributions for pairs of variables for the synthetic and real databases.

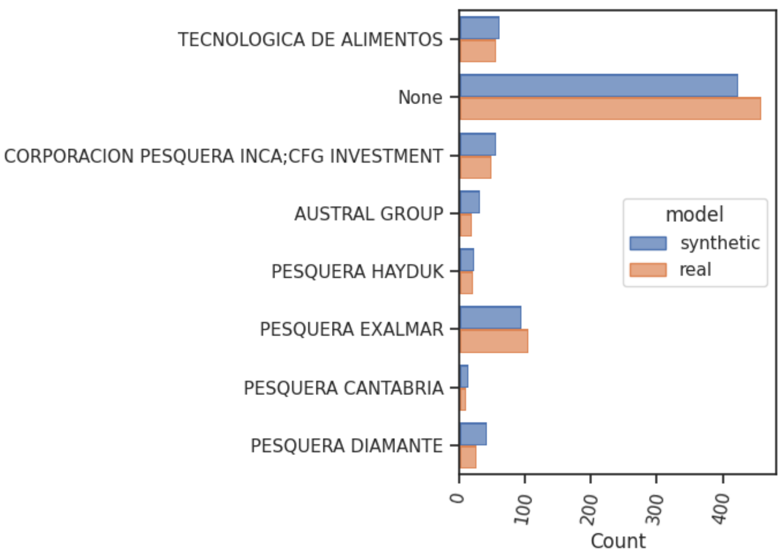


Figure 10.16: Counts of synthetic vessels in a sample of 750 that correspond to each buyer label, in comparison with the real database (i.e,. 750 vessels)

10.5.2 Capture rate estimation

Two $\mathcal{GP}$ models were fitted, one for each corresponding vessel type. For the wooden case, a performance of $R^2 = 0.88$ was obtained, while for the steel case, the performance value was $R^2 = 0.77$. In both cases, it can be observed that the model prediction describes adequately the decreasing trend of the capture rate in a fishing season (see Fig. 10.17 and 10.18). On the one hand, for the steel vessels, the predictions made on the training dataset shape a smooth curve with a standard deviation that encompasses the inter-daily variability (see Fig. 10.17). We verify this pattern when observing that the prediction a random samples in the range of $(0, 1)$ also follow this smooth curve (green 'x' in 10.17). On the other hand, for the wooden vessels, the predictions depict a curve that seems to mimic the training dataset (see Fig. 10.18). In fact, when predicting on the random sample, we observe that the curve approximates the real data on the training points, but follows a linear fashion on the rest of the curve. While this may be an indication of overfitting for the wooden vessel model, we considered that the performance was good enough given that aim was not to explain the change in capture rate, but to introduce this variability into the ABM model in a stochastic manner. Finally, we identify a correlation between high values of capture rate and days of intense fishing activity, as was shown in Fig. 10.6. We can especulate that all vessel owners have some sort of knowledge that leads them to perform an intense fishing activity during the days of high capture rate. What cannot be told is the direction of the causality: do vessels fish because the fishing rate is high? or the the fishing rate is high due to the intense activity?

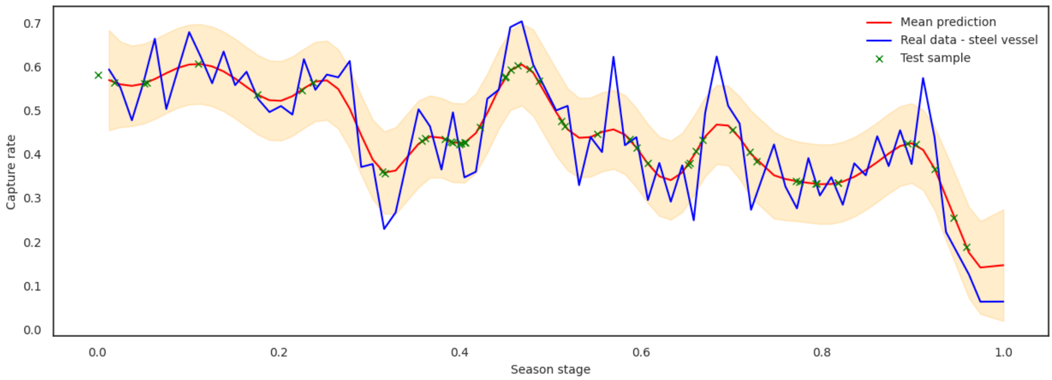


Figure 10.17: Capture rate variation of steel vessels in a fishing season (2021-1). Blue line indicates the real mean values. Red line and shaded area represent the mean of the prediction and the confidence interval (95%), respectively, evaluated on the whole dataset. Green 'x' are predictions of sampled values from $\mathrm{U}(0, 1)$.

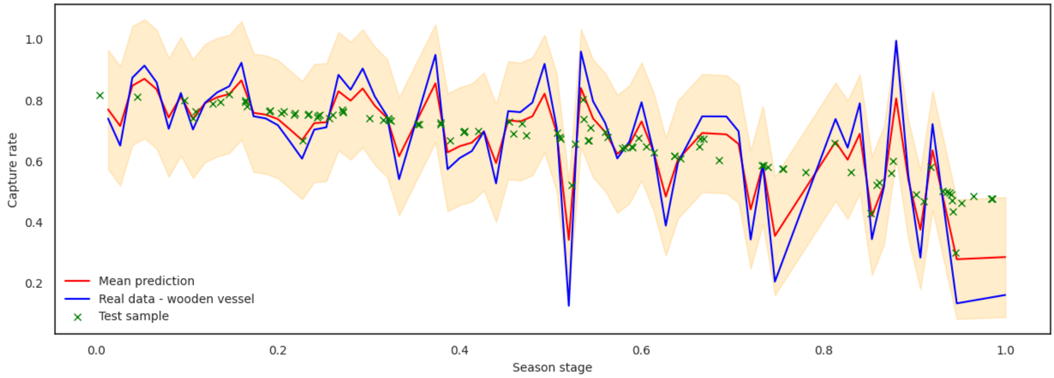


Figure 10.18: Capture rate variation of wooden vessels in a fishing season (2021-1). Blue line indicates the real mean values. Red line and shaded area represent the mean of the prediction and the confidence interval (95%), respectively, evaluated on the whole dataset. Green 'x' are predictions of sampled values from $\mathrm{U}(0,1)$.

10.5.2.1 Validation of scenario A

We first present the results of the scenario A in terms of the aggregated behavior of the model. For this, in Fig. 10.19 we show the frequency of landings per type of vessel (i.e., left axis barplot) as well as the cumulative distribution of landed anchovy (i.e., right axis curve). The red line indicates the *tac* value, while the shaded area on the curve shows the confidence interval of the Montecarlo simulations. We see that the cumulative distribution curve increases rapidly until reaching $t = 50$, and that the *tac* is almost exhausted by $t = 80$. If we compare this with Fig. 10.5, we can tell that the cumulative trend is similar to the one observed in 2029-I, although our ABM model seems to let the wooden vessels dominate the fishing activity.

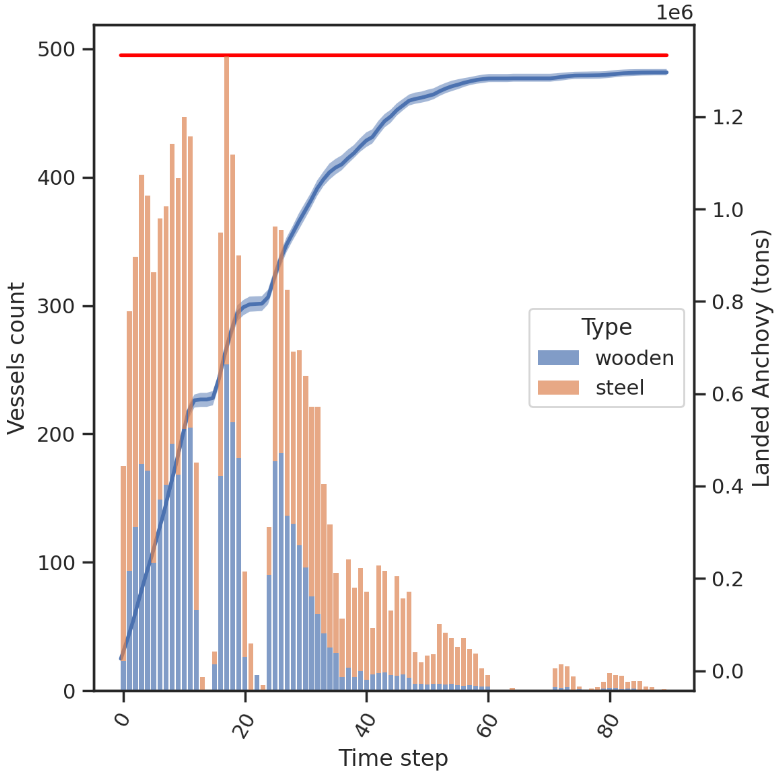


Figure 10.19: Landed anchovy accumulation (tons) (blue line) and fishing vessel counts (bars) for the ABM model of 2029-I production

With respect to impacts, we see that the life-cycle impact of a kilogram of fishmeal in the network has a mean of 0.4597 Kg CO_2eq (see Fig. 10.20). This behavior is expected since an aggregated LCA calculation of the fish meal production using ecoinvent 3.6 (see Fig. 10.11), yields a GWP impact of 0.4524 kg CO_2eq using average fleet compositions (see red line). However, two companies, AUSTRAL and CANTABRIA, stand out from the rest because of their higher and lower life-cycle impacts, respectively. This can be explained by the particular characteristics of the fleets. While AUSTRAL relies mainly on owned steel vessels, CANTABRIA depends mostly on wooden vessels, which have lower $fuel\_rate$ values. In real life, both AUSTRAL and CANTABRIA posses this kind of fleet, confirming the capacity of the synthetic data fleet to create plausible fleet samples.

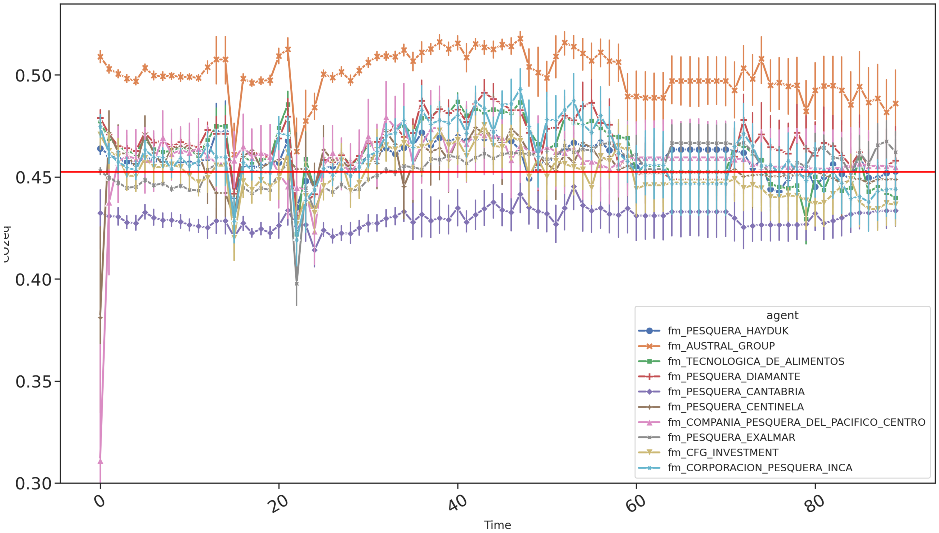


Figure 10.20: Life-cycle impacts evolution for the fishmeal industry in a simulation of the fishing season 2029-I. The vertical lines show the confidence intervals from 60 Montecarlo simulations. Red line shows impact from an LCA model using average values

Fig. 10.21 shows that the daily flow of money is varies among all the companies during the first half of the simulation, while the second half is dominated by two companies. Negative flows indicate situations were companies do not manage to sell their production, yet they keep producing since the programmed rules indicate to produce as much as possible. Eventually, they sell their inventories and reach zero after a while. With respect to the two dominating companies (i.e., EXALMAR and TECNOLOGICA), their high variability in money flow can be explained by the stochastic nature of `pacha.engine.Scheduler`. By being the only two remaining competitors in an almost satisfied market, the company selling first dominates the day. Moreover, it is important to mention that while these two companies are indeed dominant in the real world (see Table 10.3), the simulation has no rules about financial strategies or factors that cause this success. Meaning that this trend is a reflection of the ingested $capacity^p$ parameters.

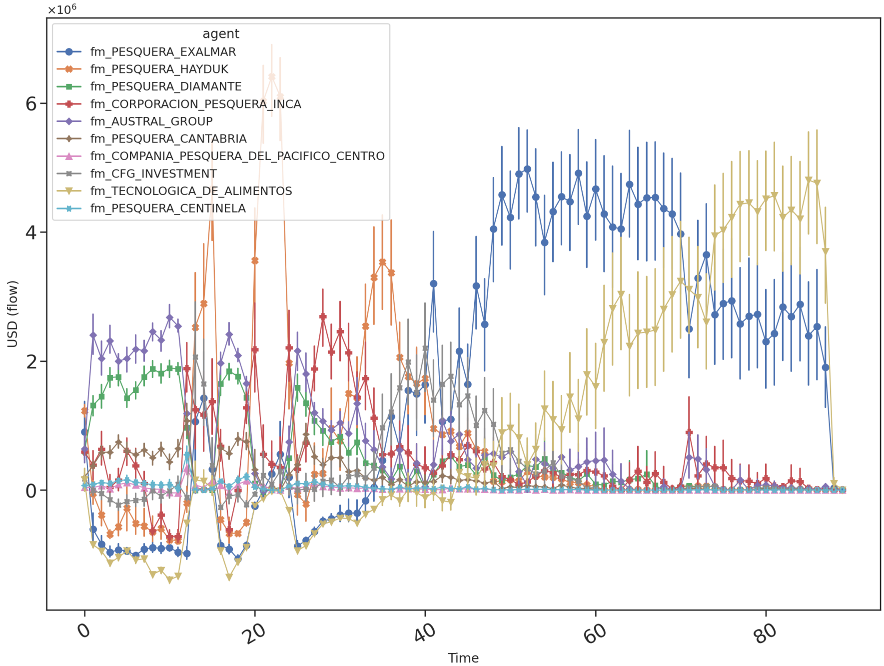
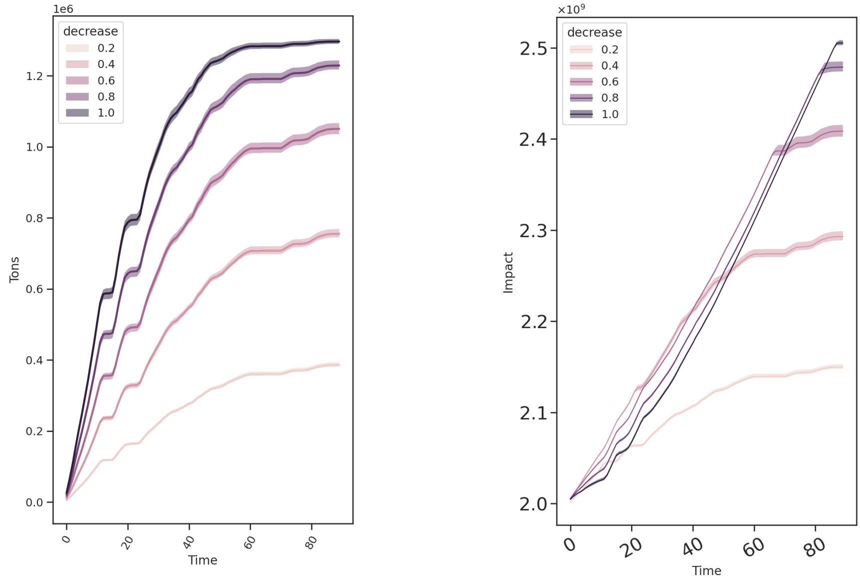


Figure 10.21: Daily money for the fishmeal industry in a simulation of the fishing season 2029-I. The vertical lines show the confidence intervals from 60 Montecarlo simulations.

10.5.2.2 Disruptive scenarios

We show the changes in landed anchovy cumulative distribution when decreasing the *decrease* factor. We observe that a proportional reduction on the availability of fish does not lead to a proportional reduction of production (see Fig. 10.22a). For a $decrease = 0.8$, the supply is reduced by 5 percent, while for $decrease = 0.2$, the supply is reduced by 70 percent. This pattern can also be observed in the money accumulation of the fishmeal producer, which is directly correlated to the supply of anchovy, since plants produce as much as they can (see Fig. 10.22b). This behavior occurs because the *decrease* factor affects the *capture_rate*, leading to a decrease in effective fishing. Since there exist an oversupply of anchovy providers, a decrease in *capture_rate* allows the participation of other vessel owner that are usually left out.



(a) a (b) a

Figure 10.22: Change in landed anchovy accumulation (a) and money accumulation (b) due to a mid-term disruption. Decrease factor modifies the capture rate.

When observing the daily money flow, we note that *decrease* provokes a change in the money accumulation pattern (see Fig. 10.23). In the case of EXALMAR, for instance, this occurs because the company does not work at full capacity anymore, meaning that they are not accumulating stock, and they just produce to sell. Moreover, this change of pattern is also observable when analysing the average life-cycle impact of the system, in which for lower values of *decrease*, a clear increase in impacts is observed (i.e., see Fig. 10.24).

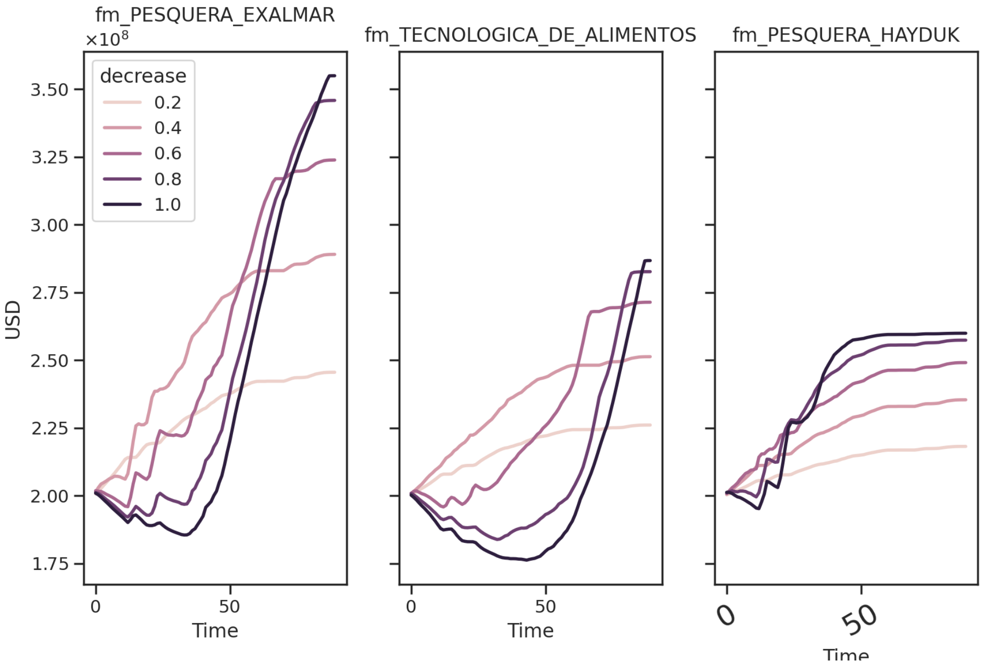


Figure 10.23: Change in daily money flow for three fishmeal companies. Decrease factor modifies the capture rate.

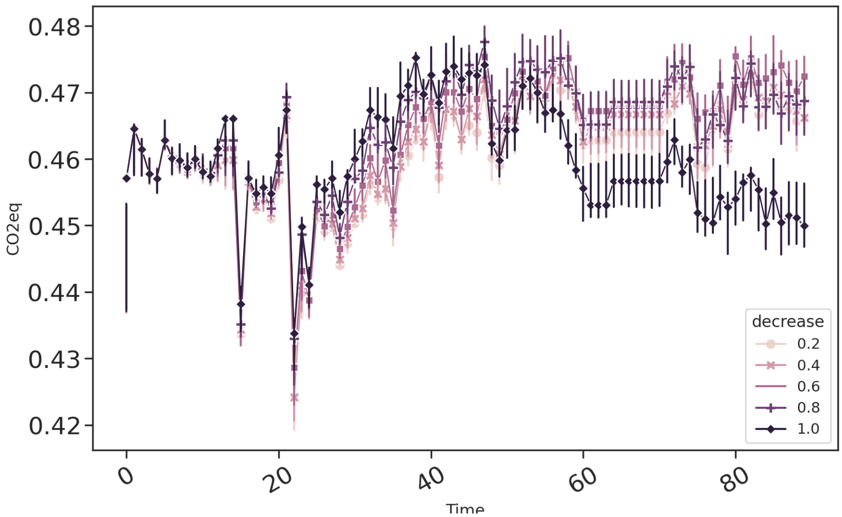
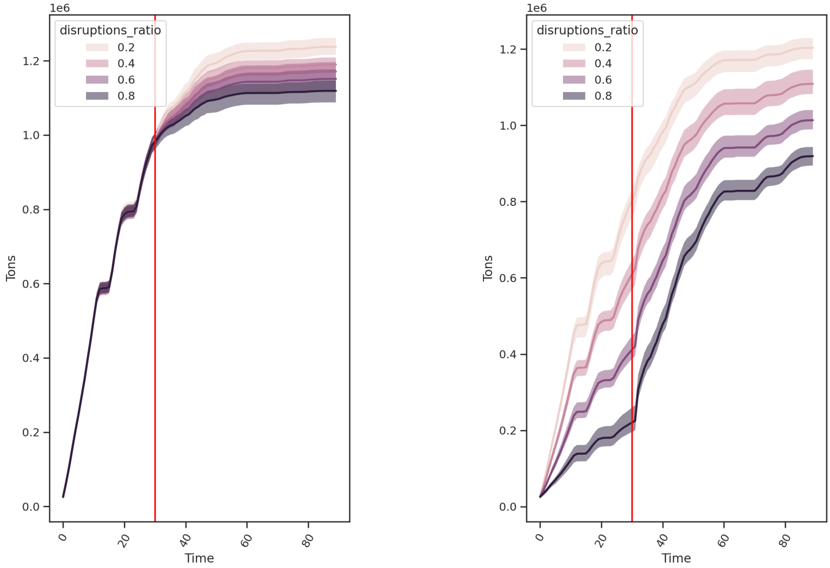


Figure 10.24: Change in the average life-cycle impact of a kilogram of fishmeal in the supply network. Decrease factor modifies the capture rate.

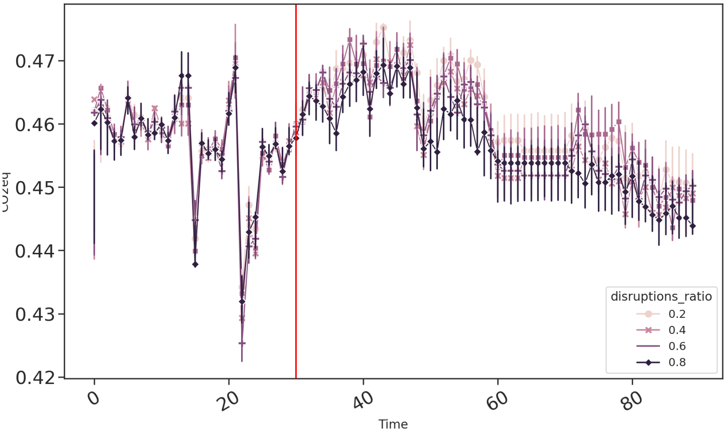
With respect to the short-term disruptions, we observe that the time frame of affectation has a relevant impact in the system performance. When selecting the $t > 30$ period, the consequences to the system are minimal since, as shown in Fig. 10.19, most of the intensive fishing occurs the first month of the simulation, decreasing considerably the remaining days (see Fig. 10.25a). Nevertheless, differently from the scenario B, the landed anchovy accumulation shows greater variability from the moment of the disruption until the end. This can be attributed to the $disrupt_t$ function which affects agents randomly, contrary to the scenario B in which all vessels were equally affected. When selecting $30 < t$, we note that this random disruption has a distinguishable effect in decreasing the accumulation rate in the period of affectation (see Fig. 10.25b). In fact, when observing $disruption\_ratio = 0.8$, we note that the accumulation has a greater change rate after the disruptions stop. Despite of this, the change rate is not enough to let the system return to normal supply, indicating a low level of resilience.



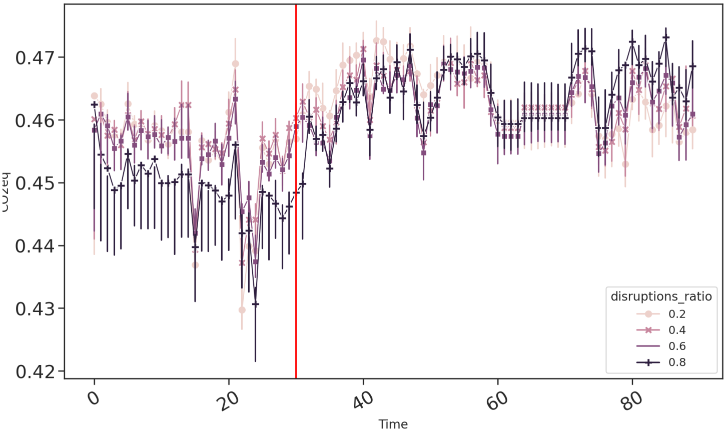
(a) (b)

Figure 10.25: Change in landed anchovy accumulation for random disruptions for t<30 (a) and t>30 (b). Shaded areas represent variability of 60 Montecarlo simulations. Red vertical line represents t=30

The selection of a time frame can also affect the LCA impact of the system. When $t > 30$, random disruptions introduce variability into the average life-cycle, but they do not change the overall trend (see Fig. 10.26a). While when $t < 30$, the average life-cycle impact varies depending on *disruption_rate* until reaching $t = 30$, when it converges to a common trend regardless of the initial state (see Fig. 10.26b). After the disruptions cease in $t = 30$, we observe that, for all *disruption_rate* values, the average life-cycle impact increases until 0.46. Regarding the final state of the system, we see that disruptions in the first period imply higher final average impact (i.e., approximately 0.46 Kg CO_2eq), while disruptions in the second and third period imply lower final average impact (i.e., approximately 0.445 Kg CO_2eq).



(a)



(b)

Figure 10.26: Change in the average life-cycle impact of a kilogram of fishmeal when random disruptions occur in t>30 (a) and t<30 (b). Red line represents t=30

Chapter 11

Summary Part III

11.1 About agents of change and propagation of sustainable business norms

We demonstrated that there exist strategies and network configurations where the adoption of an environmental friendly business norm can reduce considerably the impact of the system whilst not representing a riskier decision from a financial standpoint. More specifically, when an AOC appears randomly in the network, the probability of going bankrupt does not vary significantly if the system is dominated by profit-driven agents or by AOCs (i.e., scenarios a). We observed that AOCs situated in strategic locations can act as gates where the specific characteristics of consumer's demand are diluted and superseded by AOCs characteristics, meaning that the proposed conjecture 1 holds true only when AOCs are systematically located. Interestingly, these strategic agents can contribute in the reduction of the risk of becoming AOCs, while also increasing the environmental performance of the whole network.

While our conclusions are valid for SN with topologies similar to the adopted networks, the utility of our study is twofold. From an agent's perspective, a clear notion of the risk of adopting a particular business norm can facilitate companies' decision regarding becoming an AOC. From a system's perspective, understanding the effects that individual changes produce over the system and over other agents can aid the design of policies and strategies to boost the penetration of environmental friendly practices in an SN. For networks with different configurations and properties, we thus recommend the adoption of this complexity-oriented perspective when evaluating the promotion of sustainable behaviours among companies.

In this thesis, we presented two approaches for solving the sourcing problem: environmental optimization and monetary optimization (see Section 6.3.4). We have assumed agents to be rational entities, however, other types of decision-making models, such as bounded rationality, should also be evaluated. This is relevant for studying strategies that target human attitudes in both production and consumption side. Nevertheless, AFRICA is flexible enough to be adapted to other types of reasoning models beyond optimization, such as multi-objective optimization or bounded rationality. Finally, we identified that AFRICA can also be used to model socio-technical agents in other research questions, such as the study of resilience, rebound effects, circularity strategies or the identification of marginal suppliers in consequential LCA.

11.2 About the effects of disruptions on the sustainability of an SN

We presented an ABM model of the Peruvian fishmeal industry in which we explored the consequences that external perturbation can have in the system performance. We evaluated this performance using aggregated indicators, such as GWP, in combination with a temporal view of the system functioning and a disaggregated analysis of the SN components. We verified that our ABM implementation is capable of recreating certain system's emergent behaviors such as the accumulation of landed anchovy and TAC consumption. Moreover, model's impact accounting functioning was verified when compared to the results of an LCA of a supply chain of the same characteristics. With respect to the financial performance, the benchmark scenario could not be validated with real companies' financial information due to privacy issues. The absence of this kind of validation represents a limitation of our implementation, specially when recent events have shown that some companies considered in this study have declared bankruptcy and expect to cease operations. Using such information in further research could allow the enhancement of the ABM model since it can serve as ground truth to analyse the reliability of individual simulation results.

We used pacha to prepare a scheme of experimentation in which we explored mid-term and a short-term disruptions. We demonstrated that depending on the nature of the perturbation, the consequences on the system performance can be different. In the case of midterm disruptions, we showed that proportional stress on the resource extractors does not imply proportional shortage of fishmeal. This stress can alter the money accumulation patterns of different fishmeal producer agents, putting at risk their financial outcome. With respect to the short-term disruptions, we identified that the time frame of perturbation plays a critical role in the model. When they occur on periods of high productivity, they can produce changes from which the system will hardly recover, like the case of scenario B when the disruptions occurred in $t < 30$.

Some complex human behaviors, such as the skipper effect, are relevant since they are factors of production. However, these could not be incorporated as explicit rules in the ABM implementation because of the ontological uncertainty regarding this phenomenon. This difficulty was addressed by encapsulating this effects in machine learning models that were trained using data associated with changes in performance. Future studies focusing on the influence of fishing fleets in fishmeal production should consider an explicit modelling of these phenomena.

Our results indicate that the composition of the fishing fleet has relevant influence in the impact of the production of fishmeal, but it does not capture possible dynamics among vessel owners. While we considered fishing vessels as independent agents interacting with fishmeal producers, reality shows that vessel owners can cooperative among themselves, or even form clusters of agents to increase the efficiency of the fishing activity. This limitation can be addressed by programming explicit rules of cooperation or information diffusion among vessel owners to replicate this real behavior.

Disruptions are intrinsically a temporal dependant phenomenon, meaning that reducing this dynamic component from the assessment neglects the effects that it has on any measured impact. While it may be possible to represent affectations using some proxies (i.e., final reduction of production capacity), this still requires to be dynamically modeled to explain the impacts' evolution. Finally, we have shown that data driven approaches can be used to approximate trends or to embed behaviors when there is lack of better information. This can be convenient to add plausible variability to an unknown phenomenon in the modelling process.

Part IV

Insights and conclusions

Chapter 12

Conclusions

The need of a complexity-oriented approach capable of integrating aspects like disruptions into the assessment exercise is justified since the proper modelling of an SN is complex from different perspectives. Moreover, when exploring possible reasons for an absence of this, we identified epistemological differences in the way how practitioners interpret these concepts. This previous conceptual exploration was necessary to propose a set of foundations that should be taken into account when addressing this kind of system. The operationalization of such a theoretical framework required and effort of designing tools and methodologies accordingly, such as AFRICA and pacha. Using ABM as the core paradigm, we have shown that a complexity-oriented modelling framework can indeed enhance the assessment exercise when dealing with sustainability related inquiries. This, however, is not straightforward since ABM is not an out-of-the-box solution by its own, but it should be part of an integrated collection of concepts and tools that operate in coherent manner.

We presented two cases of study where the insights from conventional sustainability assessment methods (i.e., LCA) were enhanced by the use of a complexity-oriented approach. On the one hand, we tested some fundamental assumptions regarding the influence of green-conscious agents in systems dominated by profit-driven firms. On the other hand, we used an empirical case of study in which we simulated the effects that external perturbations can have on sustainability of the Peruvian fishmeal production industry. In the following part, we will answer the research questions proposed at the beginning of this thesis, using our conceptual development and the findings of the cases of study as support.

12.1 RQ 1: How distant are concepts like sustainability and resilience from an epistemological and ontological perspective?

We addressed this question by conducting a critical review based on a non-systematic literature search. At the best of our knowledge, this review is novel in discussing the methodological impediments and advances when modelling complex SNs and assessing their sustainability. Trends regarding modelling approaches in SN, sustainability, complexity and disruptions were also explored in order to identify relevant perspectives. Additionally, we showed that the differences in the selection of methodologies by practitioners can be influenced by differences in the motivations and the temporal scope of studies. We classified these differences in three: temporal, motivational, and methodological. This let us confirm Hypothesis 1 since both sustainability and resilience are indeed different from an epistemological point of view, however they share similar features like the survivability goal.

We have put in evidence that an appropriate assessment method that is coherent with the selected SN modelling approach is required in order to be useful in practice, whether it is for designing or for improving a sustainable SN. The necessity of considering actors' agency to achieve sustainability as an emergent norm has also been acknowledged in other studies since businesses actions respond to motivations beyond utilitarianism (Murtagh et al., 2020). While an ongoing trend on the study of disruptive effects over SNs has been observed (Bier et al., 2020; Katsaliaki et al., 2021), similar efforts to enhance sustainability assessment methods to consider complexity are still missing. Our point of view is consistent with the conclusions drawn by (Bier et al., 2020), where methods to mitigate disruptions were reviewed and a more complexity-oriented SN agenda was proposed.

12.2 RQ 2: How can modelling objectives, such as resilience and sustainability, be coupled in the same assessment exercise in coherent manner?

We suggest that sustainability assessment approaches should also evolve in a conceptual and methodological manner to consider multiple aspects of a CAS, such as resilience, adaptability and the dynamism of network's topology. We have elaborated four theoretical principles that we consider should guide the development of any complexity-driven sustainability assessment approach. The principles concur to the notions of treating sustainability as a multidimensional space, and acknowledging the relevance of time for both network's evolution and metrics selection. Under this vision, resilience objectives are embedded into the sustainability target, which can provide a common framework for analysis. These principles helped us to confirm Hypothesis 2 as a common assessment approach was possible to achieve due to these underlying principles. Moreover, we proposed an assessment framework that has been built on the basis of the proposed principles. Steps that depict data acquisition, computational modelling, sustainability region delimitation and decision-making have been outlined to portray the desired characteristics of an operational assessment method. Substantial part of the framework has been built taking stages of the conventional ABM paradigm, meaning that challenges associated with this modelling approach will also arise.

The fact that our framework relies on the delimitation of the sustainability region also represents an important challenge. Selecting the appropriate sustainability dimensions (i.e., target-oriented metrics) is not trivial, and it is a task that should be based on science, but also on understanding societal and industrial goals. Likewise, establishing sustainability boundaries requires the quantification of these limits. This may represent an issue for environmental dimensions where a consensual objective is not yet defined, or where it is difficult to allocate global targets to specific sectors (i.e., GHG emissions reduction plans). While the establishment of sustainability boundaries is conditioned by practitioners' objectives, it is still important to pay attention to the development of comprehensive and consistent sustainability metrics. The absence of established boundaries of sustainability does not hinder the use of a complexity-oriented approach. As it was shown in the cases of study, LCA-oriented metrics can still be used in the interpretation of results. In fact, the assessment of metrics on a temporal basis allows to expand the understanding of the mechanisms behind the behavior of a system.

This thesis provides a first attempt to set conceptual principles to guide the construction of CAS-oriented sustainability assessment methods, presenting ABM as the adequate tool to facilitate the future development of a methodology. Since supply systems are becoming more complex and intertwined than ever, it is important to constantly evaluate if current methodological tools are comprehensive enough to address these complex systems. In this sense, we consider that future practitioners can rely on our findings to discuss current methodologies or to provide robustness to their own approaches when assessing and modelling SNs.

12.3 RQ 3: How can SNs features, such as agency, be coupled in practice with existing tools like LCA in the same operational framework?

Based on the findings attributed to the exploration of RQ 1 and 2, we proposed AFRICA as the core operational framework for modelling socio-technical agents in ABM. This framework was a fundamental component of the operationalization of the ideas that surged in this thesis, partly because its capabilities of considering agent's technological and non-technological aspects in a computational manner. Since AFRICA treats agents as entities with inputs and outputs, many socio-technical operations that could be modeled with heuristics were modeled in an algebraic way using the same framework. In fact, AFRICA is capable of modelling adequately the operational configuration of most types of agents (i.e. producers, markets and consumers), allowing the study of conventional (i.e., impact of the system), and more complex (i.e., likelihood of survival of an AOC) sustainability inquiries.

Our framework is mathematical and language-agnostic, meaning that it can be programmed as part of any ABM simulator. To prove such statement, we developed pacha, a python package designed to provide a simulation environment for the modelling of SNs in sustainability research. pacha has a computational implementation of AFRICA, and it provides a toolkit in order to facilite experimentation and to avoid ad-hoc implementations. At the best of our knowledge, pacha is the first tool that allows to conduct ABM simulations while conducting LCA instances in the same operational framework. This package is flexible enough to be adapted to different cases of study or research question, as it was shown in the two cases of study. In conjunction, AFRICA and pacha allowed to test Hypothesis 3 because we showed that it is possible to have both ABM and LCA-methods coupled in the same operational framework.

12.4 RQ 4: What can the sustainability assessment of complex SNs gain from the use of behavioral information and ABM?

We proposed two different cases of study in which we test the capabilities of ABM as modelling paradigm for sustainability assessment. In both cases, we used our tools and methods to simulate counterfactual situations to identify the consequences that some initial conditions have on the system's sustainability. These two cases were not fortuitously selected, but they represent two streams in which sustainability research can advance, and to which this thesis contributes. The first stream is oriented to the study of fundamental questions about the sustainability of systems. In this research stream, practitioners could propose and explore theories, principles, or experiments following a rationale similar to the one used in the first case of study. The second stream is focused on enhancing the current assessment approaches by introducing agency and dynamic components into the modelling and the sustainability assessment. In this research stream, practitioners can complement their current range of tools with AFRICA or pacha in similar way as it was done in the second case of study.

In the first study, we illustrated a simulation experiment in which we observed how the environmental impacts vary when companies adopt a sustainability-oriented business norm. Thanks to the consideration of agency, we obtained insights that go beyond the product-oriented vision, such as the existence of a ratio that minimizes the risk that changing business norm may represent. In the second case of study, we showed that accumulation of impacts and its trend can vary disproportionally when unexpected disruptions are introduced. This exercise allowed us to see the capabilities of the complexity-driven approach, but also to identify caveats of current methods, such as LCA, which is a good estimator of the overall impact, but cannot easily embed notions of patterns and temporality. This case also showed that even when considering a temporal view, product's life-cycle impact trends can only indicate changes in the information shared among companies, but they cannot be used to interpret other properties of the system. Because of this, we argue that the non-linearity of certain systems can be adequately depicted by enhancing methods like LCA with other complexity-oriented methods. All these arguments can be used to test the Hypothesis 4, since our implementations of coupled ABM-LCA have provided relevant insights.

12.5 RQ: How can we assess the sustainability of an SN when it is affect by disruptions?

The sustainability of systems under disruptive effects can be addressed by incorporating a complexity-oriented perspective into the modelling exercise. This thesis presents an approach to do so, which is representing the system as a socio-technical system. In practice, this inclusion can be achieved by a combination of adopting a network perspective and providing agency to modeled entities. In this thesis we showed that incorporating complexity, both conceptually and operationally, is not trivial. Nevertheless, we provide two deliverables (i.e., AFRICA and pacha) that are designed for the modelling of socio-technical system, and have proven utility in real cases of study. We argue that these two outcomes can help in preventing the building of ad-hoc models, and they can represent the foundations of a *lingua franca* among the ABM and the LCA community.

Chapter 13

Data and code availability

Packages and code used in this manuscript are in the process open-source disclosure. The three repositories associated with this publication temporarily stored in private repositories before they are released to the public. For the anonymous reviewing process we have provided a temporal account to review, comment and replicate our experiments. Three main python3 packages were used in the elaboration of the manuscript. The simulation was built using `pacha`

Pacha, the package used for the simulation, can be found and installed using this repository: https://git.list.lu/gustavo.larrea/pacha

Repository used to run the simulation presented in the Agents of Change study in chapter 9 can be found in this repository: https://git.list.lu/gustavo.larrea/my_image_experiment

Repository used to run the simulation presented in the Peruvian fishmeal study in chapter 10 can be found in this repository: https://git.list.lu/gustavo.larrea/aeneas_fishmeal

Data resulting from simulation and used to produce images can be found in this repository: https://git.list.lu/gustavo.larrea/africa_poc_data

The repositories provided in previous section are stored in a private repository while an open-source disclosure process goes through. To access them, a temporal account is provided. After accessing the repository, it is required to be authenticated using the following information: (see Figure 13.1).

username: anonymous_reviewer_aeneas
password: Hyar9ow.

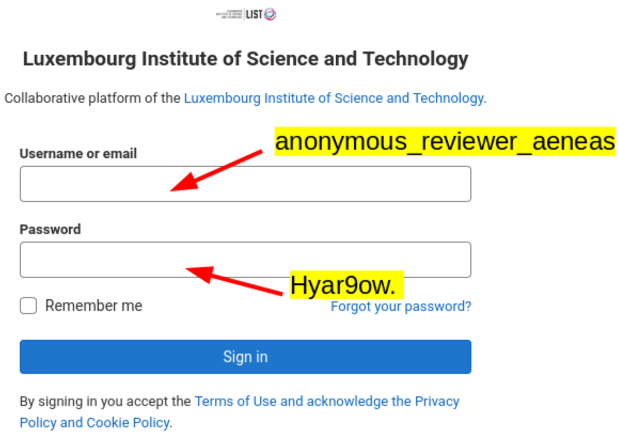

LIST
Luxembourg Institute of Science and Technology
Collaborative platform of the Luxembourg Institute of Science and Technology.
Username or email
anonymous_reviewer_aeneas
Password
Hyar9ow.
Remember me
Forgot your password?
Sign in
By signing in you accept the Terms of Use and acknowledge the Privacy Policy and Cookie Policy.

Figure 13.1

Publications

2. Larrea-Gallegos, G., Benetto, E., Marvuglia, A., & Gutiérrez, T. N. (2022). Sustainability, resilience and complexity in supply networks: A literature review and a proposal for an integrated agent-based approach. *Sustainable Production and Consumption*, *30*, 946–961
3. Larrea-Gallegos, G., Benetto, E., Marvuglia, A., & Navarrete Gutierrez, T. (n.d.-a). A computational framework for modeling socio-technical agents in the sustainability assessment of supply networks. *(under review) Sustainable Production and Consumption*
4. Larrea-Gallegos, G., Benetto, E., Marvuglia, A., & Navarrete Gutierrez, T. (n.d.-b). Understanding the sustainability of the Peruvian fishmeal industry under the effects of disruptions. *in preparation*

Dissemination

5. Larrea-Gallegos. Gustavo, Benetto, E., Marvuglia, A., & Navarrete Gutierrez, T. (2022). Using agent-based modeling to embed disruptive impacts in the sustainability assessment of supply network: a proof of concept on the Peruvian fishmeal industry. *LCAFOODS*
6. Larrea-Gallegos, G., Benetto, E., Marvuglia, A., & Navarrete Gutierrez, T. (2021). Understanding the role of disruptions in the assessment of the sustainability of a supply network. *10th International Conference on Life Cycle Management*
7. Larrea-Gallegos, G., Benetto, E., Marvuglia, A., & Navarrete Gutierrez, T. (2023b). pacha: a python ABM toolkit for simulating supply networks in sustainability research. *11th International Conference on Industrial Ecology*
8. Larrea-Gallegos, G., Benetto, E., Marvuglia, A., & Navarrete Gutierrez, T. (2023a). On the complexity of sustainable production systems: using agent-based modelling to understand the role of sustainable Agents of Change in a supply network. *SETAC Europe 33rd annual meeting*

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Appendix A

Fundamentals of LCA in Industrial Ecology

In the conventional LCA practice, the most relevant computational step corresponds to the calculation of the LCI. In this step, all the flows that are required to supply a certain amount of reference product are calculated by solving a set of equations. These operations are usually represented following the algebraic formulation proposed by Heijungs and Suh, 2002. According to this, it is required to establish a technology matrix, $\mathbf{A}$, which is an $n \times n$ matrix containing the physical flows, a_{ij}, from technology row i to technology column j, in order to produce a given unit of product j. Additionally, an environmental matrix, $\mathbf{B}$, containing the physical flows that are not inputs of any technological column must be set. The values in $\mathbf{B}$ represent the flows from the technological entities (technosphere hereafter) to the environment (e.g., CO_2). The algebraic operations become handy when the calculation of environmental and technological flows are required for a given demand $\mathbf{f}$. In this sense, the problem is formulated as follows:

given a demand $\boldsymbol{f}$*, what are the flows required from the technosphere?.*

These required technosphere flows, or technology mix, will be expressed as a supply vector, $\mathbf{s}$, and the associated environmental flows as an inventory vector, $\mathbf{g}$. The before mentioned system can be described by equation A.1, meaning that determining the flows, $\mathbf{s}$, linked to given demand f becomes an accounting problem. Since the unitary flows are described, it can be solved using linear algebra and the $\mathbf{s}$ vector can be obtained as the unknown of a system of linear equations. The system is solved using equation A.2. Finally, the inventory vector is calculated following equation A.3.

$$\mathbf{As} = \mathbf{f} \tag{A.1}$$

$$\mathbf{s} = \mathbf{A}^{-1}\mathbf{f} \tag{A.2}$$

$$\mathbf{g} = \mathbf{Bs} \tag{A.3}$$

Equation A.1 is the proper formulation of the LCA problem. It represents a system of n equations with n unknowns that can be solved by inverting the technology matrix, $\mathbf{A}$, as shown in equation A.2. This is valid for any case as long as the technology matrix $\mathbf{A}$ is square (i.e., only one input from one technology), and the assumption of 'technosphere flows only' is valid. For supply chains that are expected to be invariant in a period, this approach is convenient and have been the keystone of many LCA studies. For cases where the short-term supply chain is unknown, this approach is no longer consistent and practical. The difficulty arises when the studied system requires multiple technologies simultaneously, and the mix of technologies may vary during time. For this, Duchin and Levine, 2011 proposed a variation of the conventional input-output approach that considers simultaneous technologies called Technology-of-Choice Model (TCM). Katelh ön et al., 2016 expanded the TCM by introducing stochasticity and proposing a formalization suited for the LCA calculation (i.e., STCM). Since its proposal, the STCM has been used in different LCA studies, specially those with consequential approaches Duchin and Levine, 2011; Katelh ön et al., 2016; Kätelhön et al., 2019; Larrea-Gallegos et al., 2018.

The STCM expands the traditional square structure of the technology matrix in order to include new columns that correspond to new technologies. This implies that the new matrix is no longer square, but rectangular with $n \times m$ dimensions, and it denoted as $\mathbf{A}^*$. Despite the modification of the technosphere, the LCA question proposed in equation A.1 has not changed. However, the scaling vector, $\mathbf{s}$ (i.e., n elements), does not match anymore the dimensions of $\mathbf{A}^*$ (i.e., $n \times m$). For these, a new scaling vector $\mathbf{s}^*$ with m dimensions is proposed. The former equation A.1 is reformulated in equation A.4

$$\mathbf{A}^*\mathbf{s}^* = \mathbf{f} \tag{A.4}$$

Equation A.4 cannot be solved with matrix inversion. This is basically because the number of equations, n, is less than the number of unknowns, m, leading to an undetermined system with infinite solutions for $\mathbf{s}^*$. The STCM proposes that an unique technology mix, $\mathbf{s}^*$, can be obtained by introducing a set of criteria and restrictions, which transforms the calculation of $\mathbf{s}^*$ into a linear programming problem. In this sense, a factor matrix $\mathbf{F}$, with $k \times m$ dimensions and coefficients f_{pj}, is introduced to represent the amount required of factor p by the technology j. Additionally, a cost vector $\mathbf{k}$ and a constrains vector $\mathbf{c}$, both with k dimensions, are introduced to represent the costs and restrictions of each p factor, respectively.

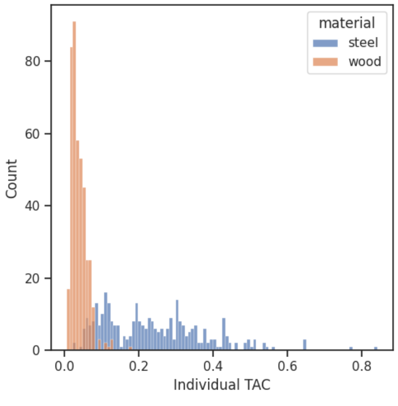
The solution of the scaling vector $\mathbf{s}^*$ is then obtained by solving the linear programming model presented in equation A.5 using restrictions set in equations (A.6) - (A.8).

$$\mathbf{min} \qquad \boldsymbol{Z} = \boldsymbol{k}^T \boldsymbol{F} \boldsymbol{s}^* \tag{A.5}$$
$$\mathbf{A}^*\mathbf{s}^* = \mathbf{f} \tag{A.6}$$
$$\mathbf{s}^* \geq 0 \tag{A.7}$$
$$\mathbf{F}\mathbf{s}^* = \mathbf{c} \tag{A.8}$$

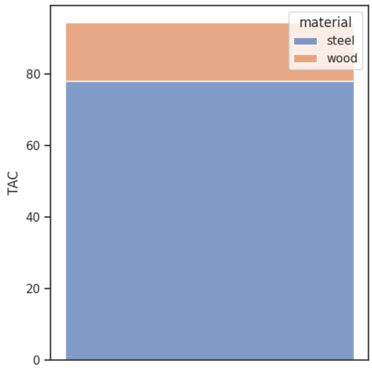
With the formalization of the computation paradigm of STCM, the practitioner's task is to build the matrices with enough and reliable information, either from primary or secondary sources. The technosphere presented in the SCTM represents the foreground processes and assumes that the practitioner knows that background flows related to the foreground technosphere. A widely used source of background information is the database ecoinvent (Wernet et al., 2016), which contains information regarding technosphere and environmental flows of many products and services across the world.

Appendix B
Figures

B.1 Anchovy landings in the first fishing season of 2019



(a)



(b)

Figure B.1: Histogram of individual TAC per hull type of the Peruvian anchovy fishing fleet (left side), and the share of accumulated TAC (right side).

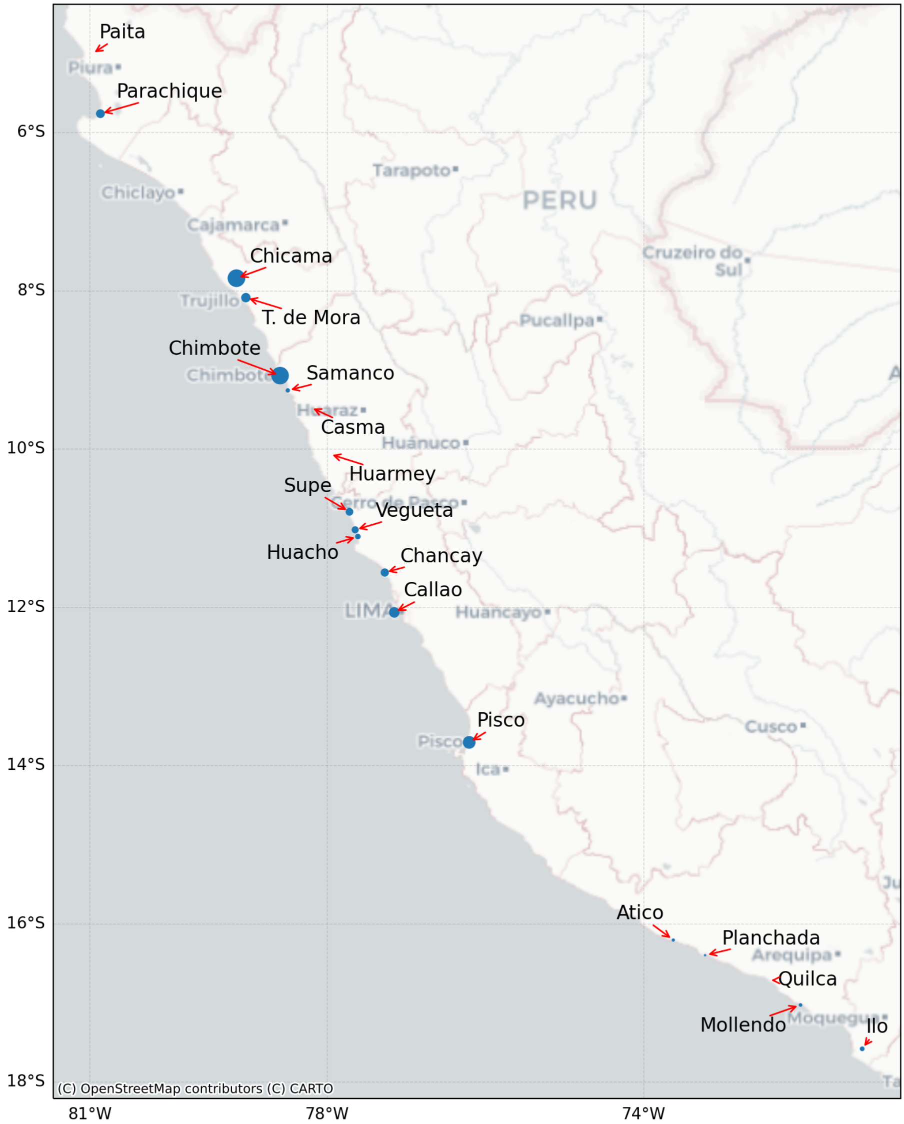


Figure B.2: Geographical distribution of anchovy processing ports in Peru.

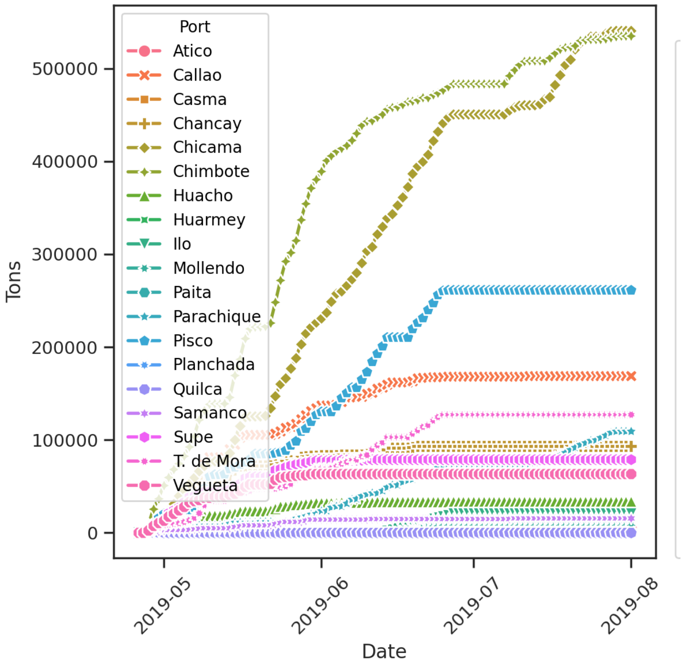


Figure B.3: Accumulated daily anchovy landings for each Peruvian port in the season 2019-1

B.2 Capture rate verification

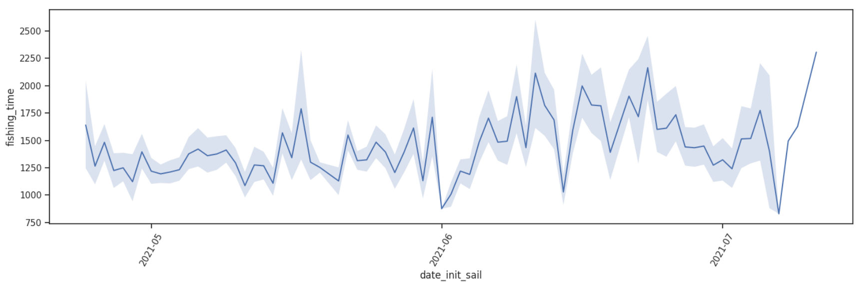


Figure B.4: fishing time variation in the 2021-1 season grouped storage capacity.

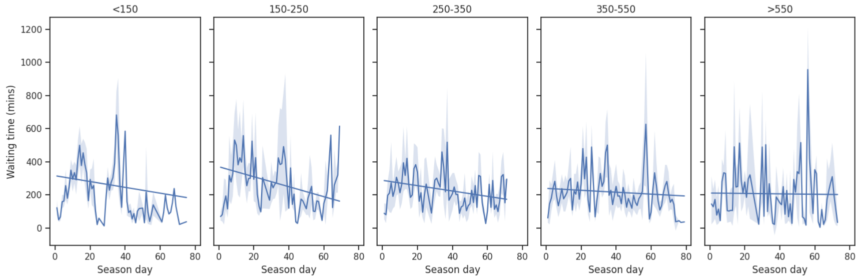


Figure B.5: Waiting time in port before landing in the 2021-1 season grouped by storage capacity

B.3 Generative model validation

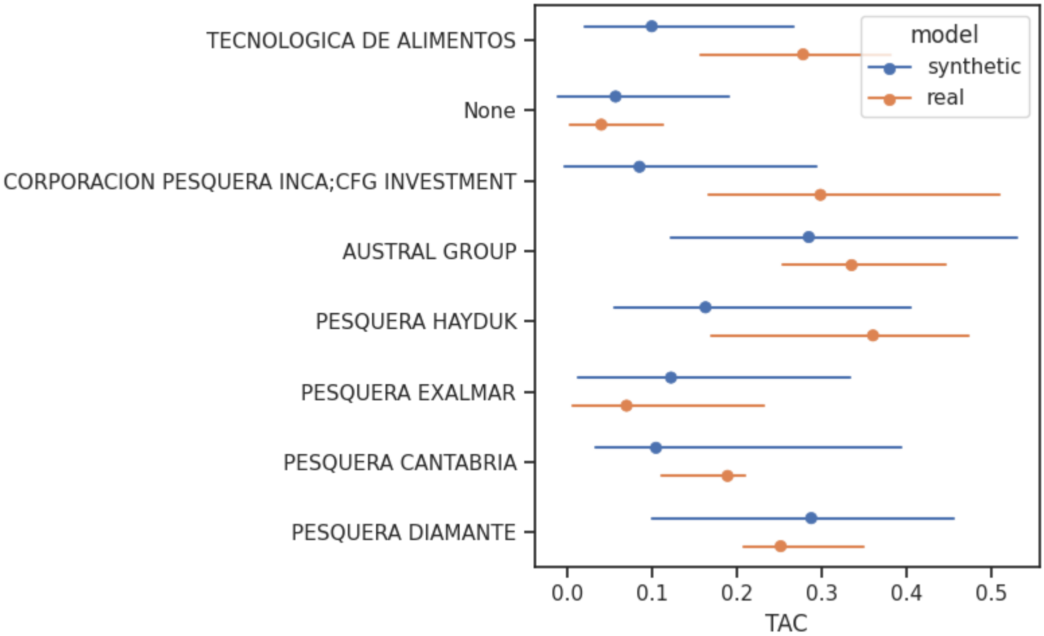


Figure B.6: Distribution of synthetic and real vessel buyers in a sample of 750 synthetic vessels.

B.4 Processing rate and market prices

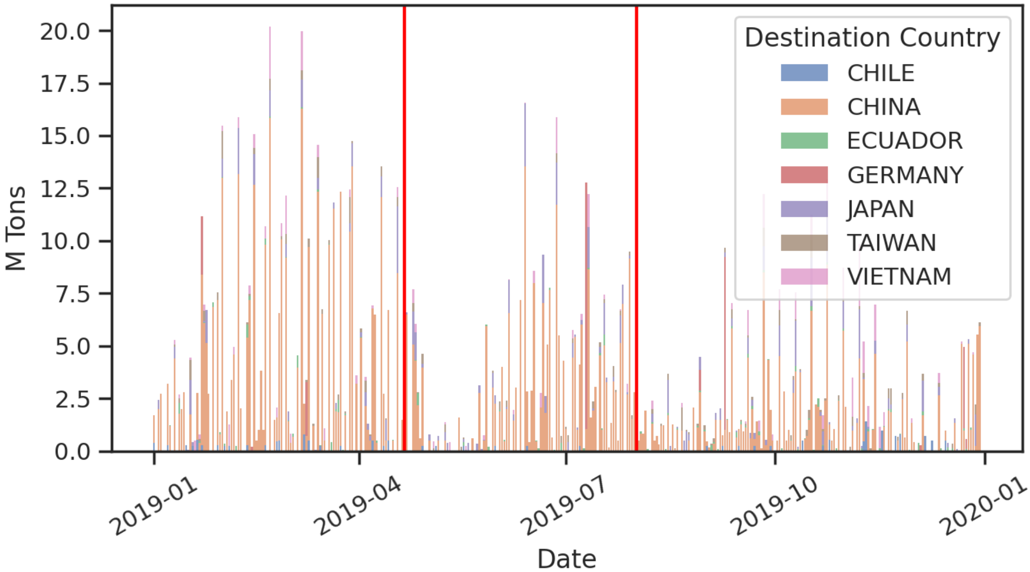


Figure B.7: Exportations of fishmeal in the year 2019. Red lines indicate the beginning and end of the first season.

B.5 Results and validation

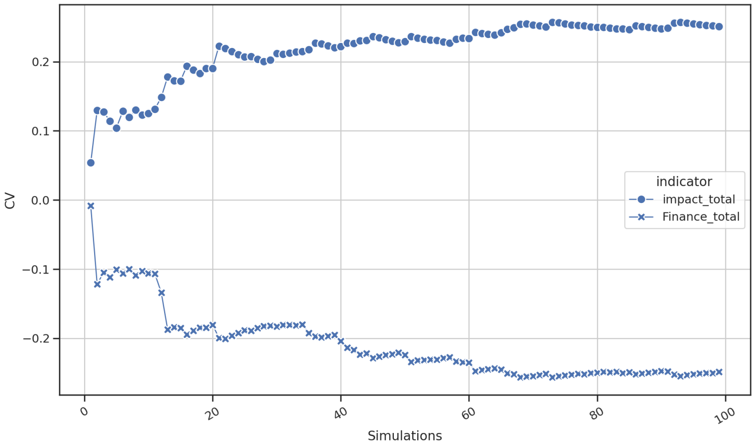


Figure B.8: Converge of the coefficient of variation, measured for the system's total impacts and total money accumulation. $\tau = 60$ was selected as number of Montecarlo simulations

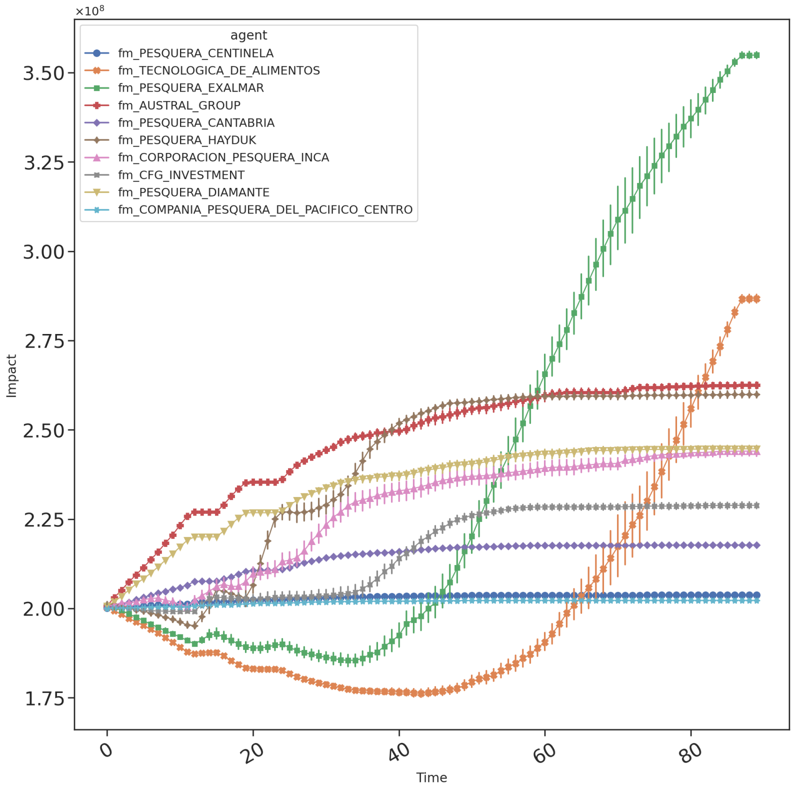


Figure B.9: Accumulation of money (USD) for each fishmeal producer in a simulation of the 2019-1 fishing season