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Learning from multi-paradigmatic sensitivity in cross-cultural management? Empirical and theoretical considerations

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Abstract

Paradigms are basic assumptions about how social reality is perceived, understood and explained. Whereas most research is based on a single paradigm, few empirical papers show the advantages of using multiple paradigms within a study. This article pleads for multi-paradigm studies in cross-cultural management research in order to reach a more multifaceted representation of cultural phenomena. This is particularly consistent with the field of cross-cultural management, because it would be ethnocentric to consider intercultural situations only from one perspective, usually that of one's own culture. The argument corresponds to the ambition of cross-cultural management to respect and adopt multiple (cultural) perspectives and, analogously, to achieve a 'paradigmatic ethnorelativism'. Based on an intercultural situation, and therefore going beyond meta-theoretical reasoning, this article demonstrates multi-paradigmatic sensitivity in terms of the functionalist, interpretive and critical paradigms. The use of these theoretical concepts leads to multiple angles and a less 'ethnocentric' position, and hence to more nuanced knowledge creation with regard to the intercultural situation. The 'blind spots' of each paradigm, but also their complementarities, are discussed. Consequently, this article raises theoretical and practical implications for cross-cultural management by offering a way to a richer understanding of intercultural situations through openness to different paradigms.

Keywords

Critical incident, cross-cultural management, ethnorelativism, international management, meta-level, multi-paradigm study, multi-paradigmatic sensitivity, paradigms, reflexivity

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Introduction

The relevance of various basic assumptions about reality is often underestimated. The continuing coexistence of these assumptions leads to parallel world views, so-called *paradigms*. Paradigms are systematic basic assumptions about how the world is perceived, understood and explained (Kuhn, 1970). Paradigms thus provide research fields with a framework, orientation points and structuring features that are used consciously or unconsciously to generate insights and explanations in the complex and contradictory (scientific) world (Burrell and Morgan, 1979; Kuhn, 1970).

In order to stimulate discussion on a reflexive meta-level, scientific paradigms should be given increased attention in research. Researchers from different disciplines often criticise each other on the basis of varying, supposedly 'wrong' or 'inappropriate' theoretical frames of reference, methodological approaches and viewpoints on research questions or the interpretation of research results. Most researchers argue that paradigms are 'mutually exclusive views of the social world' (Burrell and Morgan, 1979: iii) and in no way compatible. In this paper, we aim to show that the conscious handling of one's own preferred paradigm and especially the openness to other paradigms, called *multi-paradigm research*, make it possible to adopt multifaceted perspectives on research phenomena. This promises not only an enrichment of knowledge but also innovative outcomes.

The relatively young discipline of cross-cultural management research is affected by various 'separated' paradigms. As an analogy, these various paradigms can be compared to different cultures in intercultural situations, for example in international working contexts. We argue that in cross-cultural management it would be very one-sided to analyse these situations only from one (often one's own) cultural perspective, since a deeper understanding of a situation is not reached this way. Such ethnocentrism could correspond to a mono-paradigmatic view, which limits the respective analysis. Therefore, it would be more coherent to use multiple perspectives in an ethnorelativistic sense, and consequently multiple paradigms for knowledge creation which we call *paradigmatic ethnorelativism*. This analogy offers an argument consistent with the field and purpose of cross-cultural management – sensitivity to, respect for, and acceptance of multiple perspectives.

There are two paths that result in attention to different paradigms. First, the call for separate research works with similar phenomena in focus but different paradigmatic positions. In cross-cultural management research and practice, the dominance of a mostly quantitative – so-called *functionalist* – paradigm (concepts of Hofstede, 2001, or House et al., 2004), as well as a hermetically rigid concept of culture, is clearly given priority (Barmeyer et al., 2019b; Fang, 2012). Other researchers confirm this dominance (Barmeyer et al., 2019a; Primecz, 2020) and plead for an opening of the research field towards more comprehensive paradigmatic studies (Bjerregaard et al., 2009; Boyacigiller et al., 2004; Primecz et al., 2009; Pudelko et al., 2015; Sackmann and Phillips, 2004). A few examples extend this picture: in 2009 the *International Journal of Cross Cultural Management* published a special issue, 'Cross-cultural management research: Contributions from various paradigms' (Volume 9, Number 3), with six articles consciously selected from different paradigms. This kind of initiative creates awareness for other paradigms that can often fade into the background. Nevertheless, each of these articles was by itself mono-paradigmatic.

Second, we therefore argue for a sensitive consideration of different paradigms *within* a study of cross-cultural issues. Such multi-paradigm research in cross-cultural management is of great benefit because it allows a more diverse – ethnorelativist – view on intercultural phenomena of management and organisational practices. At the same time, this positioning of paradigm handling has a link to the solution-oriented, constructive design of cross-cultural management (Barmeyer and Franklin, 2016; Stahl et al., 2017): consciously and carefully used, the various insights that arise from paradigms contribute to research despite, but also precisely because of, their fundamentally different assumptions and thus separateness (Patel, 2016; Prasad, 2015; Primecz et al., 2015). Only a small number of existing empirical studies of cross-cultural management pursue a multi-paradigm analysis within the same (case) study (Mahadevan, 2013; Primecz et al., 2015; Romani and Primecz, 2019; Romani et al., 2011a).

This article benefits the scientific community by, *first*, pointing out the relevant theoretical concepts of three social science paradigms with regard to a concrete intercultural situation, thus highlighting the advantage of sensitivity to multiple perspectives in cross-cultural management research. *Second*, it comments on how multi-paradigm studies can contribute to the widest possible exploration of social/cultural phenomena. This combination of empirical demonstration and meta-theoretical discussion calls for more in-depth multi-paradigm studies and encourages the adoption of a reflexive meta-level. The overarching aim of our article is to direct more attention to paradigms and to raise awareness of multi-paradigmatic openness in order to derive advantages for cross-cultural management research.

The remainder of the paper is structured as follows. First, we introduce the reader to the state of the art and associated tensions in multi-paradigm studies and show briefly how we position ourselves in supporting multi-paradigm studies. We then present common social science paradigms in *organisation studies* which are being transferred to cross-cultural management research. Subsequently, we use an intercultural situation in order to show how the sensitivity to three paradigms creates a differentiated view of the situation. Consequently, the discussion will emphasise how a diversity of ways of thinking can be used complementarily to better understand the complexity of cross-cultural management – in terms of the content of the intercultural situation *and* at meta-theoretical level for proponents and opponents of this type of study. Finally, we underline the implications of this article and provide an outlook for future research.

Multi-paradigm studies: Proponents and opponents

The debate in cross-cultural management about opening up the field of research to multi-paradigm studies has its origin in various perspectives on the *incommensurability* of paradigms, meaning paradigms incompatibility due to their profound differences. These are the perspectives of isolation, integration and multiple use. The first point of view shapes the idea of *isolated* paradigms and was introduced as early as the 1970s by Kuhn (1970) and in particular by Burrell and Morgan (1979). Each paradigm is seen separately and there is and should be no possibility of combining them, since paradigms are based on incompatible ontologies, epistemologies and methodologies, and separate assumptions about human nature (Burrell and Morgan, 1979) – they are competing rather than complementary (Hassard and Kelemen, 2002: 344). Second, advocates of an *integrative* approach to paradigms are in favour of curbing ontological and epistemological pluralism and returning to a common basis in order to be able to promote (common comprehensible) knowledge (Donaldson, 1998; Pfeffer, 1993). Third, and this reflects our point of view, the *multi-paradigm* position also sees paradigms as 'separate academic worldviews' (Romani et al., 2011a: 434), but emphasises the possibility of exchange and connections between the paradigms.

Voices criticising the possibility of multi-paradigm studies have always existed. 'Isolationists' would say it's not possible to rely on different paradigms and thus it is not acceptable to relate them. Proponents of the multi-paradigm position, and we are in line with this, would argue that isolation leads to paradigm segregation and deepens analysis of only selected aspects. Moreover, Kuhn

(1970) distinguishes between three phases of science. He describes the ‘paradigm shift’ as a transition from pre-paradigmatic to ‘normal science’, saying that competing and incompatible views are largely lost over time. The scientific community can therefore accept a new paradigm. This example shows the learnability of paradigms as well as the possibility of sensitivity towards them. Additionally, ‘integrationists’ would want to come back to only one paradigm in order to enable research on a common basis (Donaldson, 1998; Pfeffer, 1993). Thus they deny the impossibility of finding a neutral common ground. In our opinion it is neither desirable to create one dominant paradigm nor is the negotiation about the ‘right’ ontology and epistemology possible any more due to the sophistication of different paradigms. Schultz and Hatch (1996: 551) referred to multi-paradigm studies as an alternative that bypasses the ‘paradigm war’ and the hegemonic position of a single paradigm, generating diversity and complementarity, and ultimately leading to novel solutions in the complex and contradictory world of knowledge as well as further reflexivity for researchers (Lewis and Kelemen, 2002; Romani and Primecz, 2019).

In our opinion, promoting the multi-paradigm position becomes particularly relevant in an intercultural context. The diverse influences of the different research disciplines of cross-cultural management could instigate multi-paradigm studies, which would underline the paradigmatic richness of cross-cultural management, discuss new paradigms, and take into account several existing paradigms in order to make the phenomenon under investigation more accessible (Primecz et al., 2009). In particular, the well-known challenges of cross-cultural management research – the strong simplification of the cultural concept, the equation of nation with culture, and the factors influencing individual behaviour that are neglected alongside the dominant cultural dimensions – can be enriched by the multi-paradigm position (Patel, 2016; Primecz et al., 2009).

Deepening cross-cultural research on the basis of one paradigmatic direction fosters *specialised* knowledge – certain aspects are perceived more sharply than others – which definitely has its *raison d’être*. Nevertheless, a progressive wider vision would achieve a conscious and constructive handling of paradigms beyond this narrow view of cultural realities and intercultural interactions; this we aim to demonstrate. Through this endeavour, similarities and differences between the paradigms come to the fore. Through differences in particular, we gain novel, complementary insights, i.e. other resulting paradigm foci and topics, which then can be examined from one’s own paradigm to gain advanced knowledge about research phenomena.

So far, there are only a few studies of cross-cultural management that pursue multi-paradigm strategies. They open up a more diverse view of interculturality and at the same time show the positive effects that a multi-paradigm study can have. For example, Romani et al. (2011a), in ‘Paradigm interplay for theory development: A methodological example with the Kulturstandard method’, illustrate the possibility of interaction between the functionalist and interpretive paradigms. The interplay shifts the focus of each individual analysis and thus helps to further develop theories and the research orientation of cultural standards. Mahadevan (2013), in ‘Performing interplay through intercultural simulations: Insights on tacit culture in a Taiwanese–German management team’, also illustrates the interaction of the functionalist and interpretive paradigms, during an intercultural simulation in a bicultural management team. The interaction of these paradigms is made possible by a reinterpretation of the functionalist GLOBE-study categories (House et al., 2004), ‘*as is*’ (what people actually do) and ‘*should be*’ (what people want, values), and helps to uncover implicit culture that is lived but not verbalised. Primecz and colleagues (2015) apply a *parallel* strategy in ‘A multi-paradigm analysis of cross-cultural encounters’. They examine the lack of service orientation in Hungary, according to Turkish migrants, on the basis of four paradigms using the same interview material. The different foci create added value and a broader, multifaceted understanding of the complex role of culture in intercultural encounters (Primecz et al., 2015: 438). A further milestone that clarifies the interplay strategy is the article by Romani and Primecz (2019), ‘Promoting and demystifying paradigm interplay: Reflexive practices on a study of Turkish mobile professionals’. While conducting the analysis, interplay was put into practice, and the authors reached different findings concerning Turkish mobile professionals’ experiences of integration in Hungary and Sweden. This ‘simultaneously reveal[s] how the interplay strategy, as a knowledge production process, is inscribed in the person, the practices, and the community of researchers doing interplay’ (Romani and Primecz, 2019: 31).

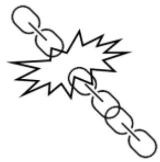
In this paper, we deal with the three main groups that classify multi-paradigm studies (see Lewis and Grimes, 1999; Lewis and Kelemen, 2002; Schultz and Hatch, 1996): first, on the basis of the *multi-paradigm review*, we present three important paradigms in organisation studies that enable researchers to orient themselves and define their own point of view – this is what we do in the section that follows. Thereafter, second, based on a critical intercultural situation, we raise sensitivity for *multi-paradigm research*, indicating which theoretical concepts would be the focus of analysis for different paradigms in order to create a more comprehensive understanding. Most important, third, in the discussion we want to contribute to *meta-paradigm theory building*. We highlight the advantages but also the blind spots of each paradigm as well as the benefits of approaching an intercultural situation from multiple paradigms. We also show those who doubt the meaningfulness of multi-paradigm studies that these studies do not generally assume that paradigms can be combined, either. Instead, a sensitive handling of the researchers’ own dominant paradigm and of other paradigms’ differences and similarities can overcome stagnation and drive progress.

Social science paradigms in cross-cultural management research

Even though the debate on paradigms is ongoing, we are convinced that the joint consideration of several social science paradigms is valuable, especially when investigating cultural phenomena. Therefore, in this paper, we encourage sensitivity towards multi-paradigm approaches. The classification of paradigms in organisation studies on which we rely has evolved since the 1970s. Various researchers have developed taxonomies of the available paradigms in cross-cultural management studies (e.g. Mahadevan, 2017; Patel, 2016; Primecz et al., 2009; Romani et al., 2018a). We adopt the terminology established in cross-cultural management research and focus on three paradigms: ‘functionalist’, ‘interpretive’ and ‘critical’. This is in line with Primecz (2020: 6), because ‘they [these three paradigms] have clearly distinctive basic assumptions, numerous publications based on the given paradigms, and there is a critical mass in the research community’. In the following we will broadly present their main features (see also Table 1).

The *functionalist* paradigm, also known as positivist or objectivist, is based on the assumption that the world exists objectively and phenomena are real so they can be measured or proven. Thus, this paradigm builds on the view that social sciences are similar to natural sciences and that models are best suited to describe social reality and to find causal relationships between social phenomena (Donaldson, 2003). *Comparative management* and the most influential stream of *cross-cultural management* belong to this paradigm (Romani, 2008: 35), based on the assumption that (national) culture is stable, has clear boundaries and is internally homogeneous. Therefore large-scale quantitative surveys search for cultural differences or similarities and thus create cultural dimensions which rely on values, or patterns of behaviour (Hofstede, 2001; House et al., 2004). One goal of functionalist management research is to support decision-makers, leading to

Table 1. Characteristics of paradigms (based on Deetz, 1996: 199 and Romani et al., 2018a: 255).

	Functionalist	Interpretive	Critical
Pictorial representation	1 + 1 = 2		
Typical request	Impact of national culture on management practices	Identification of cultural meanings used at work	(Re)production of power imbalances using cultural differences in management
Problems to be addressed	Inefficiency, disorder	Meaninglessness, illegitimacy	Dominance, consent
Social anxiety	Disorder	Depersonalisation	Authority
Basic objectives	Relationships between objects are rule-oriented and structured	Identification of patterns of common meanings	Demasking of power
Basic mood	Optimistic	Kind	Suspicious
Investigation procedure	Extensive quantitative studies and questionnaires	In-depth qualitative methodological and ethnographic studies	Critical discourse analysis and critical ethnography
Contributions to cross-cultural management	Culture becomes measurable and comparable, dominance of/major impact on management	Emic and local knowledge, context-rich understanding of interactions	Hidden power structures that play a role in dealing with culture and cultural differences

the increased effectiveness and efficiency of their organisations. Consequently, the current social order is not questioned.

The *interpretive* paradigm focuses on the understanding of culture through the explanation of social order 'from within a culture' (Romani, 2008: 6). Cultures are seen as interpretive frameworks (Geertz, 1973). Actors are sense-makers, because they perceive the socio-cultural reality within their interpretive frameworks in different ways and therefore give particular meanings to their social reality (Romani et al., 2011b). This paradigm thus pursues a subjective basic attitude. Corresponding studies therefore search for possible interpretations and social constructions of realities from the actors' viewpoints (D'Iribarne, 2009). To study culture and intercultural interactions, context plays a decisive role: 'The context is our content' (Jackson, 2019: 1). The use of language as a core element of a meaning system also plays a crucial function (Holden, 2008). Research questions attempt to clarify differences and similarities between views of interest groups and thus describe and explain the respective attributed meanings from the actors' perspectives (e.g. Gertsen and Zølner, 2014; Zølner, 2019). Observed phenomena, rather than laws, are represented. It is assumed that social and organisational phenomena are constantly changing, and that reality is always constructed and reconstructed by the actors. Concepts such as leadership, feedback and performance are culturally subjective (Chevrier, 2009). Consequently, concerning the socially constructed phenomena of research interests, 'only' the subjective interpretations made by the researcher (active role) are possible in this paradigm.

The *critical* paradigm (Alvesson, 2002; Mahadevan, 2017), which also includes the *postcolonial* paradigm (Jack and Westwood, 2006), considers knowledge and cognition as the result of a reflexive *process* of investigation. Dating back to Max Horkheimer, Theodor Adorno, and Herbert Marcuse, the ideological critique of capitalist societies is the subject of traditional critical theory. Alvesson and Willmott (1992) transferred these ideas to management studies. Critical research attempts to explore social phenomena through social inequality, injustice, dominance and exploitation. It takes into account those actors who have 'less power' and are less considered in social science. Disagreements concerning the existing (hidden or visible) social order and its power structures are uncovered, which leads to discussions. Cross-cultural management often focuses on power imbalance issues such as gender or religion in the workplace (Romani et al., 2018b) and intersectionality (Mahadevan et al., 2020). The aim of this iterative, reflexive approach is to improve society morally (Deetz, 1996: 202) or, in cross-cultural management, intercultural interactions and thus interpersonal relationships.

Multi-paradigmatic sensitivity: A critical incident illustration

To demonstrate the advantages of multi-paradigm research and in line with Jackson's (2011: 535) request 'to develop scholarship that can handle context-dependent, pragmatic action-oriented diversity', we have chosen a *critical incident* (Flanagan, 1954), an intercultural situation characterised by typical misunderstandings and conflicts (Batchelder, 1993). These are triggered by cultural differences (e.g. diverging norms and value systems) and misinterpretations (e.g. diverging attributions of meaning) of the behaviour of the interaction partners.

The case was not collected within the framework of classical empirical social research but as part of a consulting assignment by the co-author of this article. It serves to illustrate how the same intercultural situation could be addressed by different paradigms, the *functionalist*, *interpretive* and *critical* paradigms. Diversity is highlighted, and paradigmatic differences are featured. We are able to show that multi-paradigmatic sensitivity leads to various angles on a specific situation and its context and thus a more differentiated understanding of the situation.

Self-reflexively, we, the authors of this article, are aware that due to our scientific socialisation we also express a preference for certain paradigms in our analysis. We situate ourselves at the interface of the functionalist and interpretive paradigms. Critics often ask for a clearer positioning of the researcher's own paradigm while conducting multi-paradigm studies. This is due to the fact that one's own dominant paradigm influences the way one sees and writes about the different paradigms. Moreover, being neutral or writing a paper solely from a meta-perspective is impossible. Multi-paradigm researchers have noticed that addressing only one audience at a time is advantageous in order to avoid confusing the readers (Romani et al., 2011a). We have chosen functionalist language at this point because it is most common in cross-cultural management and thus reaches a larger audience, not because we give priority to the paradigm in general.

The critical incident in Box 1 occurred in a German multinational company, a chemical group with subsidiaries in 30 countries worldwide including France. The financial department of the German headquarters is responsible for preparing the consolidated balance sheet. For this purpose, it requires the corresponding balance sheet figures from the foreign subsidiaries. Now, as when the incident occurred (in 2010), corresponding data is requested internally via email. The communication is mainly done in English, but sometimes also in German, depending on the language competences of the foreign colleagues. As is often the case in large corporate structures and across national borders, the actors do not know each other personally. Similarly, the parent company generally expects the subsidiaries to respond quickly. However, the French subsidiary did not reply.

Box 1. A French–German critical incident.

Just a formality?

A French controller (female) sends a French subsidiary's half-year figures to her colleagues in the German parent company for the preparation of the balance sheet for the entire group.

A few days later she receives an email from a German colleague (male), written in German: "Dear Ms. Dupont, thank you very much for sending me the key figures. Unfortunately, the numbers you sent are wrong. Please check them again. Yours sincerely, Manfred Müller'."

The French controller is irritated and a little bit angry: first, the figures are not wrong from her point of view, and secondly the message seems very rude to her. She feels her honour has been offended. She blocks and does not answer her German colleague. He waits . . . and waits – no answer from France. Nevertheless, the consolidated balance sheet must be prepared.

In order to demonstrate multi-paradigmatic sensitivity and the benefit of using multiple angles and perspectives, the following question arises: *What concepts and theories exemplify possible analytical foci of the functionalist, interpretive and critical paradigms?*

Functionalistic analysis

Concepts of intercultural research, such as cultural dimensions (Hall, 1981; Hofstede, 2001) or cultural standards (Thomas, 2018), are typical in the functionalist paradigm and are used to contrast cultural differences. Being sensitive to this paradigm, in this part we focus intentionally on national culture, which is typical for the functionalist mindset and its favouring of the tangibility of universal concepts, facts and figures.

Misunderstandings or problems arising in intercultural situations are often explained by *cultural dimensions*. In the present case, the masculinity/femininity cultural dimension defined by Hofstede (2001) could be used as a possible explanation for this critical incident. Masculinity characterises a society in which the roles of the different genders are clearly delineated: men have to be tough and materially oriented; women must be more modest and sensitive and value quality of life. Femininity characterises a society in which the gender roles overlap: both women and men should be modest and sensitive and attach importance to quality of life (Hofstede, 2001: 297). Masculine value orientations thus relate to characteristics such as independence, determination, initiative, achievement and competition, whereas feminine value orientations relate to harmony, equality and solidarity (Table 2).

From a functionalist point of view and in terms of Table 2, the short and firm German email lacks personal address ('Management as manège') and thus can be seen as a 'masculine' orientation, which may have aggrieved the French colleague who is used to more empathy ('Management as ménage'). The French colleague is more relationship-oriented, expecting an email to start more softly and indirectly with a few personal questions or remarks. According to Hofstede (2001), the difference of the femininity orientation of French people and the high masculinity of Germans explains the misunderstanding of such employees.

Another cultural dimension that could be used to explain the conflict is that of the cultural anthropologist Edward T Hall (1981). He describes whether people in communication situations tend to express their concerns more explicitly, i.e. clearly and distinctly, or more implicitly, i.e. indirectly and with paraphrasing. In the context of intercultural communication situations, Hall raises the question of information transfer and understanding: how much information (quantity) has

Table 2. Key differences between femininity and masculinity cultural dimensions (Hofstede, 2001: 299 and 317, extract).

Femininity	Masculinity
Relationship orientation	Ego orientation
Work in order to live	Live in order to work
Sympathy for the weak	Sympathy for the strong
Management as ménage (soft)	Management as manège (directive)
Expected use of intuition, feelings, seeking consensus	Expected to be decisive, firm, assertive, aggressive, competitive, just

to be passed on in which form (written/oral) and in which way (explicit/implicit), by whom (sender), to whom (receiver), in which language? Hall argues that people from France tend to communicate implicitly, whereas people from Germany tend to be more explicit. The German versus the French communication style is a national difference frequently discussed in cross-cultural management (Barmeyer et al., 2019b) and other studies (Heidenreich et al., 2012). In our case, the directly criticising email of the German employee is an explicit communication that may have offended the French counterpart.

Concerning written and oral communication it is important to underline that in Germany oral communication is perceived in the professional context as fleeting, imprecise and intangible, whereas written communication is considered to be precise and important; it can be relied upon and be enforced in the long term. This is also expressed in German everyday sayings such as 'Wer schreibt, der bleibt' ('Those who write, stay'). In contrast, in France, written communication is perceived as impersonal and anonymous. It is therefore classified as less important than oral communication. An important message tends to be conveyed personally (Hall, 1981). The French employee in our case would have preferred personal dialogue, e.g. a telephone call, over an impersonal written email.

Cultural standards, nearly unknown in English-speaking literature with a few exceptions (Brueck and Kainzbauer, 2000; Romani et al., 2011a), are defined by Thomas (2018) as ways of perceiving, thinking and evaluating, and the typical actions of members of the same social system. Thomas (2010) identifies central cultural standards for Germany such as *factual orientation* (dealing with facts is more important than dealing with people), *directness* (expressing opinions clearly and unambiguously using necessary facts) and *separation of personality and life areas* (separation of professional and private life). While, according to Thomas (2018), German culture attaches great importance to objectivity in communication and cooperation, French culture is more person-oriented. In Germany, the relatively pronounced masking of feelings and moods enables efficient communication and cooperation. On the other hand, the quality of relationships in France increases by building personal trust and thus contributes significantly to efficient communication and cooperation. In our case, the fact-oriented email of the German colleague could be explained from a functionalist point of view, with German cultural standards offending the person-oriented French colleague.

In a nutshell, we summarise what kind of knowledge is reached: the functionalist paradigm focuses on 'objective' knowledge. The aim is to contrast and explain German–French cultural differences that lead to intercultural misunderstandings. Existing concepts, such as cultural dimensions, are used for this purpose. It is therefore about external and generalising knowledge that can be applied in an etic way to different intercultural situations.

Interpretive analysis

Researchers who assign themselves to the interpretive paradigm will immediately ask for more context regarding the critical incident because they search for perspectival perception. They would want to know about the sense-making process of involved actors – how notions and patterns of behaviour are perceived and interpreted differently. This is based on the assumption that within cultures actors develop and use specific systems of meaning which enable them to communicate and cooperate meaningfully with each other (Brannen, 2004; D'Iribarne, 2009; D'Iribarne et al., 2020). In our critical incident, different systems of meaning come together and lead to irritation because one actor (mis) interprets the behaviour of the other. In order to raise awareness and sensitivity to the interpretive paradigm, we use the following common interpretive theoretical conceptualisations in the field of cross-cultural management to show corresponding characteristics of an interpretive analysis: recontextualisation, negotiated culture, discourses and narratives (Gertsen and Zølner, 2020).

Recontextualisation describes the process of transferring practices as well as values from one country context to another, for example from parent company to subsidiary. To enable meaningful reception, meanings need to be adapted to the target context (Brannen, 2004; Gertsen and Zølner, 2012). In our case, an interpretive researcher could identify the failed transfer and try to capture the lack of understanding based on associated meaning in the German and French contexts respectively.

Another concept used in the interpretive paradigm is that of *negotiated culture*, which refers to a 'new' emerging working culture through situational and context-specific interaction (Brannen and Salk, 2000). Existing cross-cultural management research already examines Franco-German interpersonal interactions and negotiation (Barmeyer and Davoine, 2019). In our critical incident, negotiation fails due to denial of dialogue, no more emails are replied to and the process is stopped. An intervening researcher (action research) could promote a future constructive joint working culture on the basis of interviews by reflecting on the respective diverging views of the colleagues concerned.

Discourses and *narratives* would be suitable, for example, to learn how the two actors of the critical incident talk about the situational sequences 'to show how managers and employees make sense of their cross-cultural experiences and how they use culture in this process' (Gertsen and Zølner, 2020: 39). The different systems of meaning and interpretation of the German colleague and the French would thus become particularly clear, including their interests, points of conflict, and aspirations. So how do the actors see and interpret the behaviour of their counterpart? For example the direct and short email from the German colleague, using no paraphrasing or courtesies, may be interpreted by the French colleague as rude or even aggressive. Which interpretation do I give to the word 'wrong' in the phrase 'unfortunately, the numbers you sent are wrong'? Are the numbers I delivered really incorrect? Or is it about something else, which is not linked to the numbers but perhaps to the quality of the relationship I have with my German colleague? Why is the message not formulated in a more polite and personal way? And why is the email written in the German language? On the other side, how may the non-reaction of the French colleague be interpreted by the German colleague? Perhaps my French colleague is ill or on holiday (personal reason)? Maybe she has not received my email (technical reason)? Perhaps she does not want to answer me (strategic/tactical reason)? It is possible that both colleagues will probably not even consider an intercultural interpretation.

Another approach in the interpretive paradigm is the consideration of national cultures. This is because culture is described as 'shared meaning' (D'Iribarne, 2009), conceptualised as 'frames of intersubjective meaning structures' (Gertsen and Zølner, 2020: 34). This presupposes close connections between actors. However, since a national culture comprises many people and thus interest (sub)groups, the 'lowest common denominator', i.e. the connection and the shared meaning system, is difficult to grasp (D'Iribarne, 2009: 311). D'Iribarne (2009) nevertheless finds underlying national unifying meaning systems, which he transfers to management systems. In empirical-emic studies, he points to historically rooted assumptions underlying national management practices. Other researchers (e.g. Chevrier, 2009; Segal, 2009), inspired by D'Iribarne, use other countries to show that culturally specific and emic understandings of supposedly universal concepts, such as leadership, empowerment or quality, are subject to different attributions of meaning and interpretation. This in turn reflects the existence of a national–cultural shared meaning. In our critical incident, these nation-specific peculiarities may also lead to misunderstanding. It is precisely this shared meaning that seems not to exist between the two actors. According to D'Iribarne (2009: 314), shared meaning also represents a 'basic concern' that people worry about or want to protect themselves from in everyday situations. As the French colleague does not respond to the email, she thus 'plays dead' – in French 'Faire le Mort'. This term is frequently used in French working life to express displeasure or even resistance. Displeasure is not verbally expressed in a conversation or in a written email, but implicitly through non-verbal behaviour. This also goes along with the national core concern of the French in relation to their job, 'métier' (D'Iribarne, 2009), which stands for the rights that come with a social position. If these rights and duties of the job are externally questioned, 'Faire le Mort' may be a possible universal response.

In a nutshell, we summarise what kind of knowledge is reached: the interpretive paradigm is about understanding the respective views on a situation of the interacting people – the subjective knowledge that the actors construct socially. It is therefore not about whether the actors' respective sense-making is right or wrong. It is about emic, culture-specific knowledge, for example forms of communication and cooperation. This knowledge is contextualised and cannot simply be transferred to other contexts.

Critical analysis

Being sensitive to the critical paradigm in cross-cultural management means demasking power imbalances and the unilateral assertion of interests, as intercultural studies from Moore (2016) and Ybema and Byun (2009) demonstrate. Mahadevan and colleagues (2020) assume that culture, power and diversity categories are interwoven and hence inseparable. Power is an integral part of any intercultural situation. In order to increase sensitivity to the critical paradigm, we detect different power asymmetries in our critical incident which we associate with three established aspects of general critical management studies that are important for the critical cross-cultural management research agenda (Romani et al., 2018b): denaturalisation, emancipation and reflexivity.

In contrast to the previous two paradigms, the critical paradigm wants to question and actively change the existing social order (Burrell and Morgan, 1979). Corresponding researchers are not considered as 'bystanders' but as 'activists' (Romani et al., 2018a: 253). The naturalised, taken-for-granted order is thus *denaturalised*. Not empathy and understanding but problematisations of knowledge come to the fore, enabling alternative research questions to generate new knowledge (Romani et al., 2018b). In terms of cross-cultural management, national–cultural differences and the well-known concept of cultural dimensions are questioned. Critical cross-cultural management considers other aspects – 'implicit power elements' (Romani et al., 2018b: 410) – influencing the perception of cultural differences independent of national culture. The paradigm thus aims to draw attention to alternatives and silenced voices (Jack and Westwood, 2009).

In our critical incident, for example, the power asymmetry between parent and subsidiary could be addressed by this paradigm from two perspectives. On the one hand, the email of the German colleague from the parent company may be seen as an expression of power and superiority by the French colleague. The person from the 'powerful' parent company can *place* demands and the person from the 'powerless' subsidiary should *meet* the demands as fast as possible. Also, the pre-established sensation of 'correctness' and 'competence' may be associated with the 'big' German parent company, whereas the 'mistake' and the 'error' is associated with the 'small' French subsidiary. According to Perlmutter's (1969) publications on multinational enterprises (MNEs) and their strategies for managing foreign subsidiaries, this would be in line with an *ethnocentric*, powerful and regulatory parent company strategy.

However, on the other hand, a completely different perspective could also be taken which reverses the frequently stressed dominance of 'powerful' parent companies. In our critical incident, it is revealing to draw attention to the employee in the French subsidiary who, by not reacting, demonstrates power. The employee in the German parent company is dependent on the French colleague because he needs the key figures of the French subsidiary to prepare the consolidated balance sheet. However, since the French employee 'plays dead', the German colleague cannot exercise power over her. Sociological case studies in multinational companies address this hidden exercise of power (Geppert and Dörrenbächer, 2014). They show how employees in subsidiaries develop tactics and strategies to avoid complying with the guidelines of the parent company, for example because they consider them meaningless or simply because they do not want to carry out certain tasks and responsibilities. Particularly in the context of multinational companies, whose different country units are characterised by spatial, institutional, linguistic and cultural distance (polycentrism), subsidiaries can assert their interests unwaveringly against the parent company.

The inclusion or *emancipation* of less-established subjects is also reflected in further research interests of the critical paradigm. Romani et al. (2018b: 410) call these research foci 'critical diversity markers', and they include race, ethnicity, religion, language and gender. The two latter ones can be demonstrated in our critical incident: the German colleague writes his email to the French colleague in German, i.e. in the language of the country of the parent company, which can be understood as an expression of power (the email could instead have been written in English or French). Moreover, the employee in the parent company is a man, the employee in the subsidiary a woman. The socially attributed gender discrimination may be an annoyance to the French woman, even though the male German colleague may not have intended this. The direct and harsh tone of his email may emphasise *her* hurt feelings. As some women might expect, the careful handling of this woman's sensitivity is ignored by the male colleague. Seen from another angle, in contrast this could be an indicator of *his* perception of equal position independent of gender.

Often, critical researchers refer to colonialist structures and the imposition of ideas and concepts from the Western world in power asymmetries (Alvesson and Willmott, 2012; Mahadevan, 2017; Primecz et al., 2015). So the paradigm ascribes a major role to contexts, for example historical, institutional, political or economic forces. According to critical cross-cultural management, these are aspects that are hidden behind the label 'cultural differences' (Romani et al., 2018a: 254) and influence intercultural communication, as our critical incident shows. Historical (war) experiences can play a role by unconsciously negatively influencing Franco-German intercultural cooperation via negative stereotypes. These past events are anchored in both collective memories by feelings of inferiority and superiority.

Sensitivity to this paradigm necessarily involves *reflexivity* regarding basic assumptions and routines as well as the researcher's own role in the research process. It is important for knowledge generation that researchers are mindful of which of their own interests influence them (Jack and Westwood, 2009; Mahadevan, 2017). In this case, researchers would have to ask themselves whether they are more inclined towards one or the other 'superiority', depending on, for example, which nation they come from, which organisational side (parent–subsidiary) they work for, whether they are women or men themselves, but also how they approach the research process, and what the corresponding goal is.

In a nutshell, we summarise what kind of knowledge is reached: the critical paradigm is concerned with inequalities in society, and researchers of this paradigm actively seek to point out these injustices. Consequently, the critical paradigm and the created knowledge focus on the outcome of power imbalances and oppression. Ultimately, this knowledge about problems in society aims to draw attention to the imbalances, to foster change as well as identify alienation or forms of emancipation.

Discussion

Setting the paradigms in relation to each other

In this article, we demonstrate multi-paradigmatic sensitivity on the basis of a critical incident. In the following, we summarise insights gained during the juxtaposing of the three paradigms. Martin (1992: 5) postulates on the separate, parallel view of paradigms:

> What is to be learned from culture research is, in part, the usefulness of preserving the differences between these social scientific perspectives and deepening, rather than eradicating, the conflicts among them.

Differences and conflicts between paradigms should therefore be deliberately highlighted. This provides researchers with further analytical glimpses in adopting perspectives that surprise. In order to extend this statement from a *constructive* paradigm angle, complementarity can be created precisely when many views emerge through which new aspects, further discussions and various interpretations influence the research process. In this way, social reality can be presented in a more multifaceted way.

We want to highlight the following advantages and disadvantages of each paradigm presented:

The functionalist paradigm mainly concentrates on national–cultural differences which serve as explanations for misunderstandings and conflicts between the German employee and the French. An advantage is a *clear* and very accessible categorisation on the basis of cultural dimensions and cultural standards. Moreover, the knowledge about others' and one's own culture(s) is expanded. A disadvantage can be superficiality and narrowing, which is caused by boxed-in thinking. Focusing on only the French and the German *national* culture leads to the disregard of other subcultures, such as professional cultures or organisational cultures, which are rarely the focus of functionalist studies (Primecz et al., 2009: 270). These cultural concepts can increasingly be used as preparation and thus facilitators for future intercultural interactions. The blind spot of this paradigm is context-specific explanations, because the 'objective' researcher adopts an external perspective and corresponding etic methods that overlook local understanding.

The interpretive paradigm takes the specific Franco-German context into account as well as the divergent viewpoints and meaning systems of the employees. Therefore, the interpretation according to employees' own cultural imprint that assumes what is right, normal and appropriate, results in misunderstandings and conflicts. An advantage of this paradigm is not the classification of cultural differences (functionalism), but the consideration of a diversity of perspectives due to different social sense-making processes which explain individual positions and expectations. A disadvantage can be the often absent possibility of generalisation since the social sense-making processes of the actors are often context-bound and thus very (situation-)specific. Moreover, accepting specific, context-bound interpretations may lead to a blind spot with regard to the etic dimensions. Only particular, not universal, knowledge is gained.

The critical paradigm explains misunderstanding and conflict on the basis of power inequalities. Its advantage is uncovering subcultural inequalities (gender, organisation, language etc.). The awareness of conflictual power relations may give a voice to the unheard, seemingly ‘powerless’ or ‘marginal’ individuals. Thus established structures can be challenged, and power can be differently allocated, producing change. A disadvantage may be the unilateral critical world view creating a focus on society as a place of struggle. The focus on silenced voices and oppression leads to a blind spot with regard to potential or existing cohesion and consensus.

In sum, the functionalist paradigm explains the conflict through cultural differences, the interpretive paradigm through different attributions of meaning to context and behaviour, and the critical paradigm through power (in)equalities. Table 3 displays the multifaceted knowledge gains which complement existing specialised studies that rely on only *one* paradigm. Multi-paradigm analyses are not necessarily superior but simply have another aim: not to delve deeply but to widen the picture, to broaden the views on social phenomena via multiple angles. Furthermore, we believe that in general conducting multi-paradigm studies enlarges possible perspectives. Therefore, we want to invite researchers to make the effort to engage in multi-paradigmatic sensitivity from time to time.

Table 3. Multifaceted knowledge gains through paradigm analysis.

	Functionalist	Interpretive	Critical
Explanation for misunderstanding/ conflict	Cultural differences	Differences in meaning	Differences in power
Topics addressed	National culture especially, but also subculture(s)	Sense-making and systems of meaning	Power relations
Advantage	Clarity of categorisation; knowledge expansion regarding other and own culture(s)	Perception and understanding of different positions and expectations due to contextualised social sense-making processes	Revealing inequalities; making manipulations clear
Disadvantage	Narrowing through boxed-in thinking: Focus on national culture(s) and subculture(s) (organisational, professional etc.)	Lack of generalisation, as social sense-making processes are often context-bound and situation-specific	Narrowed view, because society is seen only from the perspective of struggles and seemingly flawed (power) structures
Blind spot	Emic, context-specific explanations	Etic dimensions	Cohesion and consensus
Solution found	Knowledge from cultural concepts facilitating the understanding of future intercultural interaction and acting adequately	Learning that one’s own perception isn’t always equal to others’ leads to more empathy in intercultural situations	(Unjust) power structures are identified which may entail change

Becoming open to complementary handling of paradigms in cross-cultural management research

We are not claiming that we are able to change our core assumptions, nor that it is possible 'that social scientists can adopt other positions so wholeheartedly that they determine their entire research outlook' (Parker and McHugh, 1991: 452). In their criticism of a multi-paradigm study by Hassard (1991), Parker and McHugh, furthermore, state that acting 'as if' is also not possible:

> Paradigms cannot be like spectacles that we can change when necessary, otherwise all debate between them would be reduced to academic play. There would be no point in debate since we would all be able to move between paradigmatic positions whenever we wished. (Parker and McHugh, 1991: 452f.)

But why should this not be possible? If we as researchers are informed about the debate and know about the different basic assumptions of the paradigms, we could, at least, be open and sensitive to them. It has to be clear that of course one's own paradigm has an influence, and representatives of each particular paradigm would make more profound remarks. We postulate that multi-paradigm studies are beneficial, even if one's own paradigm is influential and analyses are not perfect due to a lack of expertise in every paradigm. This is shown in the paradigmatically sensitive handling of our critical incident. While reading, didn't you, as the reader, experience 'aha moments' every now and then, and the feeling of being steered in directions you wouldn't have thought of? Isn't it surprising how many novel insights you can get even in such a short critical incident where little context is given?

In addition, the critics Parker and McHugh (1991) point to the meta-level, namely that Hassard's discussion on the four paradigms in use – four because he divides the critical paradigm into its two origins on the basis of Burrell and Morgan (1979) – goes back to 'claiming priority over the other four [paradigms] and suggesting that his discourse synthesises the discourse produced by the other four [paradigms]' (Parker and McHugh, 1991: 453). This was also criticised by Chia (1996: 40) with regard to Burrell and Morgan's 2×2 paradigm matrix: 'The question then arises of their ability to be both within the framework and at the same time in a privileged position to frame it'. Parker and McHugh (1991) introduced another argument, which is even more profound: Hassard's study is not multi-paradigmatic at all, because no 'mental gymnastics' is necessary to follow it. In our opinion, these types of critiques may have their justification, but aren't they going too far if we don't want to stagnate in terms of knowledge production? We, as a research community, could continue to argue on this level and isolate paradigms, but then there will be no progress: at most a deepening of scientific-theoretical determination and the discussion's specialisation. Especially within cross-cultural management as an applied science, it is important to activate interdisciplinarity and to argue practically:

> For Hassard, paradigms also remain distinct, if negotiable, language games whose dynamic lies primarily in the production, rather than the consumption, of knowledge spaces. (Hassard and Kelemen, 2002: 345)

This is why we come back to the analogy that was explained in the introduction: the multi-paradigmatic sensitivity demonstrated in this article goes beyond our own dominant paradigm and thus leads to a more comprehensive insight of the situation under study by possible conceptual directions. Analogically this means transferring to questioning one's own culture in intercultural situations and putting oneself in the place of the interaction partners. Empathy and ethnorelativism are appropriate keywords here. Possible motives for behaviours and underlying values of the interaction partners, but also one's own, become apparent. Reflexivity allows for stepping back to the meta-level and thus for a more diverse and no longer one-sided creation of knowledge and a better understanding of the situation.

Occasionally researchers could try to change perspectives in order to discover new insights, even if the discussion of scientific theory reaches deeper, and for some researchers our positioning would be seen superficially as an 'anything goes' approach (Feyerabend, 1975). Nevertheless, we think there is 'the need to move beyond paradigms by adopting a "pragmatic" perspective' while preserving 'the internal logic and identity of paradigms' (Hassard and Kelemen, 2002: 345f.). Critics of multi-paradigm studies are invited to try this, but are also welcome to remain fundamentally critical, so that the paradigms do not become too blurred. The scientific community might take care that multi-paradigm studies do not become a standard of mixing paradigms without reflection. Multi-paradigm studies should therefore only take place with a certain amount of reflexivity on the debate and, accordingly, on one's own paradigm. This makes a study less susceptible to being exposed as 'non-consumer', referring to 'those researchers who may not be aware of the debate on paradigms, and/or do not make it explicit in their writings' (Hassard and Kelemen, 2002: 341).

Empirical and meta-theoretical contribution

The contribution of our article is threefold. First, it should be noted that although there is literature on the methods and meaningfulness of multi-paradigm studies, few actually carry them out and *apply* them. Respective research therefore often only takes place on a meta-theoretical level (Gioia and Pitre, 1990; Schultz and Hatch, 1996). Beyond these meta-theoretical considerations, we point out different paradigm views on a critical incident, leading to a paradigmatically aware and broadened, multifaceted view on the situation. We are able to show that paradigms not only determine *what* is researched, but also *where* problems are seen and in *which way* these problems can be directed. Searching for similarities and differences enables a *constructive approach to paradigms*, which enriches research and practice accordingly through complementarity. There might already be enlightening moments as, reading through the different paradigms, aspects come to light that broaden one's own way of thinking. There is an expansion of corresponding considerations and thus the 'tunnel vision' of one's own paradigm is diminished.

Furthermore, second, we analogically demonstrate how meaningful multi-paradigmatic sensitivity can be, especially with regard to the *intercultural component* of the critical incident. In line with cross-cultural management, we show that the different perspectives gained by this sensitivity extend the possible options for successful intercultural cooperation. This is equivalent to the concept of *ethnorelativism* (Bennett, 1993) to better understand other cultural social systems and thus promote complementary cooperation. An increasing awareness and dealing with the diversity of existing paradigms in cross-cultural management leads to a *constructive* ethnorelativist attitude. In line with constructive cross-cultural management, this awareness of different paradigms – *paradigmatic ethnorelativism* – thus also enriches the field and transforms stagnation and bias into innovation (Barmeyer et al., 2019b). Without the openness to other paradigms, the picture remains mostly one-sided, exclusive and ethnocentric.

Third, the multi-paradigm approach makes it possible to repeatedly assume a *meta-level* – here not to be confused with the meta-theoretical level. A meta-level is a superordinate, intellectual-abstract view that people adopt in order to view structures, objects and interactions from a distance and thus better understand and question them. The concept originates in psychology (Metzger, 1999) and is addressed in systems theory (Luhmann, 1995) in connection with self-referentiality. The German sociologist Simmel (1908) addressed the significance of objectivity as 'freedom', helpful in understanding 'the Other'. The use of meta-perspectives makes it possible to reflect interculturality – in theory and practice – and thus to adopt a ethnorelativist attitude mentioned above (Bennett, 1993; Hoopes, 1981).

Implications, outlook and future research

Theoretical implications

Members of the research community could increasingly look at paradigms in order to learn to empathise with their own and other paradigms and thereby advance research through original findings that can enhance innovative discussions. Sensitivity to multiple paradigms means being able to present and understand research findings more comprehensively in relation to situations or phenomena. The – so far – predominantly missed opportunity of expediently and advantageously using different paradigmatic views can be taken up in cross-cultural management research by analysing complex intercultural contexts from the point of view of different paradigms. Different insights can only be gained if the existing paradigmatic diversity of perspectives is used *thematically, methodically* and *empirically* and the potential is not simply recorded on a meta-theoretical level. In addition to the discussion about multi-paradigm studies and novel possibilities on a theoretical level, further contributions with regard to empirical data and actual sensitive *application to intercultural topics* are needed.

Practical implications

The practical implications underline the advantages of knowing our own and other existing paradigms. First, multi-paradigm analysis, or even just the sensitivity to it, enables managers to reflect on cross-cultural situations from different angles and so is an eye-opener, expanding their views by making them see what they did not realise or imagine before. These actors can thus be inspired to think 'out of box' and find (innovative) solutions. Second, via a sensitive multi-paradigm mindset, managers take the ethnorelativist meta-level which helps to achieve a tendentially more neutral position. The adoption of the meta-level perspective, i.e. ultimate awareness of multiple paradigms, is addressed in publications on intercultural competence (Spencer-Oatey and Franklin, 2009) and cultural intelligence (Earley et al., 2006). This puts managers, consultants and trainers in a position to act integratively, connecting and mediating in organisational networks. In conclusion, managers familiar with paradigms tend to be more interculturally competent in concrete cross-cultural situations because they can communicate and cooperate in a targeted and appropriate manner.

Outlook and future research

The handling of multiple paradigms is still in its infancy. We wanted to demonstrate an enlightening moment: the recognition of a possibility of building up a more diverse knowledge and thus a more comprehensive understanding. From our constructive cross-cultural management point of view, researchers might focus on complementarities resulting from differences. A researcher with another dominant paradigm would probably have approached this paper differently. There will always be different points of view to be heard and discussed in the interests of knowledge generation. This is why the goal, demand and obligation of the research community might be to shift from the meta-theoretical level to empirical action using multiple paradigms or simply multi-paradigmatic sensitivity to research phenomena to generate knowledge via content. Nevertheless, the dialogue and critical debates about raising theoretical issues help to keep the balance through reflexivity.

Since every person and thus every researcher is shaped by different life stories and, therefore, different influences, the *conscious* handling of paradigms in articles must always be critically questioned. What are the basic assumptions used by the researcher? In this context, it would be extremely interesting for future studies to assemble a research team with team members from different paradigms, who would then consider a research phenomenon separately, ideally empirically, and subsequently enter into an exchange. Contrary to what we have been able to show in this paper, this team composition would first lead to a deepening of each paradigm through expert knowledge *and* then to a broadening due to the exchange about the different analyses.

This article not only strengthens multi-paradigmatic consciousness, generates attention and stimulates research discussion, but also triggers a *momentum of its own*. Respecting and actively dealing with other paradigms contributes to changing one's own awareness of diverse (previously hidden) topics and creates complementary insights on several levels. Like Lewis and Grimes (1999: 687), we would like to conclude fruitfully with the following quotation from Popper (1970: 86):

> I do admit that at any moment we are prisoners caught in the framework of our theories; our expectations; our past experiences; our language. But we are prisoners in the Pickwickian sense: if we try, we can break out of our framework at any time. Admittedly, we shall find ourselves again in a framework, but it will be a better and a roomier one; and we can at any moment break out of it again.

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References

Alvesson M (2002) *Understanding Organizational Culture*. Thousand Oaks/London/New Delhi: SAGE.

Alvesson M and Willmott H (1992) On the idea of emancipation in management and organizational studies. *Academy of Management Review* 17(3): 432–64.

Alvesson M and Willmott H (2012) *Making Sense of Management: A Critical Introduction*. London: SAGE.

Barmeyer C and Davoine E (2019) Facilitating intercultural negotiated practices in joint ventures: the case of a French–German railway organization. *International Business Review* 28(1): 1–11.

Barmeyer C and Franklin P (2016) *Intercultural Management. A Case-based Approach to Achieving Complementarity and Synergy*. New York, NY: Palgrave Macmillan.

Barmeyer C, Bausch M, and Moncayo D (2019a) Cross-cultural management research: topics, paradigms and methods – a journal-based longitudinal analysis between 2001 and 2018. *International Journal of Cross Cultural Management* 19(2): 218–44.

Barmeyer C, Davoine E, and Stokes P (2019b) When the "well-oiled machine" meets the "pyramid of people": role perceptions and hybrid working practices of middle managers in a bi-national organization – ARTE. *International Journal of Cross Cultural Management* 19(2): 251–72.

Batchelder D (1993) Using critical incidents'. In: Gochenour T (ed), *Beyond Experience. The Experiential Approach to Cross-Cultural Education*. Yarmouth: Intercultural Press, pp. 101–12.

Bennett MJ (1993) Towards ethnorelativism: a developmental model of intercultural sensitivity. In: Paige RM (ed), *Education for the Intercultural Expérience*. London: Intercultural Press, pp. 21–71.

Bjerregaard T, Lauring J, and Klitmøller A (2009) A critical analysis of intercultural communication research in cross-cultural management: introducing newer developments in anthropology. *Critical Perspectives on International Business* 5(3): 207–28.

Boyacigiller N, Kleinberg J, Phillips M, et al. (2004) Conceptualizing culture. Elucidating the streams of research in international cross-cultural management. In: Punnett BJ and Shenkar O (eds) *Handbook for International Management Research*. Ann Arbor: University of Michigan Press, pp. 99–167.

Brannen MY (2004) When mickey loses face: recontextualization, semantic fit, and the semiotics of foreignness. *The Academy of Management Review* 29(4): 593–616.

Brannen MY and Salk JE (2000) Partnering across borders: negotiating organizational culture in a German-Japanese joint venture. *Human Relations* 53(4): 451–87.

Brueck F and Kainzbauer A (2000) Cultural standards Austria-Hungary. *European Journal of Cross-Cultural Competence and Management* 1(2): 73–104.

Burrell G and Morgan G (1979) *Sociological Paradigms and Organisational Analysis: Elements of the Sociology of Corporate Life*. London: Heinemann.

Chevrier S (2009) Is national culture still relevant to management in a global context? The case of Switzerland. *International Journal of Cross Cultural Management* 9(2): 169–84.

Chia R (1996) The problem of reflexivity in organizational research: towards a postmodern science of organization. *Organization* 3(1): 31–59.

Deetz S (1996) Describing differences in approaches to organization science: rethinking Burrell and Morgan and their legacy. *Organization Science* 7(2): 191–207.

D'Iribarne P (2009) National cultures and organisations in search of a theory: an interpretative approach. *International Journal of Cross Cultural Management* 9(3): 309–32.

D'Iribarne P, Chevrier S, and Henry A (2020) *Cross-Cultural Management Revisited. A Qualitative Perspective*. Oxford: Oxford University Press.

Donaldson L (1998) The myth of paradigm incommensurability in management studies: comments by an integrationist. *Organization* 5(2): 267–72.

Donaldson SI (2003) Theory-driven program evaluation in the new millennium. In: Donaldson S and Scriven M (eds) *Evaluating Social Programs and Problems: Visions for the New Millennium*. Mahwah: Erlbaum, pp. 109–41.

Earley PC, Ang S, and Tan JS (2006) *CQ. Developing Cultural Intelligence at Work*. Stanford: Stanford Business Books.

Fang T (2012) Yin Yang: a new perspective on culture. *Management and Organization Review* 8(1): 25–50.

Feyerabend P (1975) *Against Method*. London: New Left Books.

Flanagan J (1954) The critical incident technique. *Psychological Bulletin* 51(4): 327–58.

Geertz C (1973) *The Interpretation of Cultures*. London: Fontana Press.

Geppert M and Dörrenbächer C (2014) Politics and power within multinational corporations: mainstream studies, emerging critical approaches and suggestions for future research. *International Journal of Management Reviews* 16(2): 226–44.

Gertsen MC and Zølner M (2012) Recontextualization of the corporate values of a Danish MNC in a subsidiary in Bangalore. *Group & Organization Management* 37(1): 101–132.
Gertsen MC and Zølner M (2014) Being a ‘Modern Indian’ in an offshore Centre in Bangalore: cross–cultural contextualisation of organisational identification. *European Journal of International Management* 8(2): 179–204.
Gertsen MC and Zølner M (2020) Interpretive approaches to culture: What is interpretive cross-cultural management research? In: Szkudlarek B, Romani L, Caprar DV, and Osland JS (eds) *The SAGE Handbook of Contemporary Cross-Cultural Management*. Thousand Oaks/London/New Delhi: SAGE, pp. 34–50.
Gioia D and Pitre E (1990) Multiparadigm perspectives on theory building. *Academy of Management Review* 15(4): 584–602.
Hall ET (1981) *Beyond Culture*. New York: Anchor Books.
Hassard J (1991) Multiple paradigms and organizational analysis: a case study. *Organization Studies* 12(2): 275–99.
Hassard J and Kelemen M (2002) Production and consumption in organizational knowledge: the case of the ‘Paradigms Debate’. *Organization* 9(2): 331–55.
Heidenreich M, Barmeyer C, Koschatzky K, et al. (2012) *Multinational Enterprises and Innovation: Regional Learning in Networks*. New York/London: Routledge.
Hofstede GH (2001) *Culture’s Consequences: Comparing Values, Behaviors, Institutions, and Organizations Across Nations*. Thousand Oaks/London/New Delhi: SAGE.
Holden NJ (2008) Reflections of a cross cultural scholar: context and language in management thought. *International Journal of Cross Cultural Management* 8(2): 239–51.
Hoopes DS (1981) Intercultural communication concepts and the psychology of intercultural experience. In: Pusch MD (ed) *Multicultural Education. A Cross-Cultural Training Approach*. Chicago: Intercultural Press, pp. 9–38.
House RJ, Hanges PJ, Javidan M, et al. (2004) *Culture, Leadership and Organizations: The GLOBE Study of 62 Societies*. Thousand Oaks/London/New Delhi: SAGE.
Jack G and Westwood R (2006) Postcolonialism and the politics of qualitative research in international business. *Management International Review* 46(4): 481–501.
Jack G and Westwood R (2009) *International and Cross-Cultural Management Studies. A Postcolonial Reading*. London: Palgrave Macmillan.
Jackson T (2011) From cultural values to cross-cultural interfaces: Hofstede goes to Africa. *Journal of Organizational Change Management* 24(4): 532–58.
Jackson T (2019) Editorial: cross-cultural management: the context is our content. *Journal of Organizational Change Management* 19: 247–49.
Kuhn T (1970) *The Structure of Scientific Revolutions*. Chicago: University of Chicago Press.
Lewis M and Grimes A (1999) Metatriangulation: building theory from multiple paradigms. *Academy of Management Review* 24(4): 672–90.
Lewis M and Kelemen M (2002) Multi-paradigm inquiry: exploring organizational pluralism and paradox. *Human Relations* 55(2): 251–75.
Luhmann N (1995) *Social Systems*. Stanford: Stanford University Press.
Mahadevan J (2013) Performing interplay through intercultural simulations: insights on tacit culture in a Taiwanese–German management team. *International Journal of Cross-Cultural Management* 13(3): 243–63.
Mahadevan J (2017) *A Very Short, Fairly Interesting and Reasonably Cheap Book about Cross-Cultural Management*. Thousand Oaks/London/New Delhi: SAGE.
Mahadevan J, Primecz H, and Romani L (2020) *Cases in Critical Cross-Cultural Management: An Intersectional Approach to Culture*. New York/London: Routledge.
Martin J (1992) *Cultures in Organization*. Oxford: Oxford University Press.
Metzger W (1999) *Gestalt-Psychologie. Ausgewählte Werke aus den Jahren 1950 bis 1982*. Frankfurt a.M.: Waldemar Kramer.

Moore F (2016) Flexible identities and cross-border knowledge networking. *Critical Perspectives on International Business* 12(4): 318–30.

Parker M and McHugh G (1991) Five texts in search of an author: a response to John Hassard's 'Multiple paradigms and organizational analysis'. *Organization Studies* 12(3): 451–56.

Patel T (2016) Promoting multi-paradigmatic cultural research in international business literature: an integrative complexity-based argument. *Journal of Organizational Change Management* 29(4): 599–629.

Perlmutter H (1969) The tortuous evolution of the multinational corporation. *Columbia Journal of World Business* 4(1): 9–18.

Pfeffer J (1993) Barriers to the advance of organizational science: paradigm development as a dependent variable. *Academy of Management Review* 18: 599–621.

Popper KR (1970) Normal science and its dangers. In: Lakatos I and Musgrave A (eds) *Criticism and the Growth of Knowledge*. Cambridge: Cambridge University Press, pp. 51–58.

Prasad A (2015) Beyond positivism. Towards paradigm pluralism in cross-cultural management research. In: Holden N, Michailova S and Tietze S (eds) *The Routledge Companion to Cross-Cultural Management*. London/New York: Routledge, pp. 198–207.

Primecz H (2020) Positivist, constructivist and critical approaches to international human resource management and some future directions. *German Journal of Human Resource Management: Zeitschrift für Personalforschung* 34(2): 124–47.

Primecz H, Romani L, and Sackmann S (2009) Cross-cultural management research: contributions from various paradigms. *International Journal of Cross Cultural Management* 9(3): 267–74.

Primecz H, Romani L, and Topçu K (2015) A multi-paradigm analysis of cross-cultural encounters. In: Holden N, Michailova S and Tietze S (eds) *The Routledge Companion to Cross-Cultural Management*. London/New York: Routledge, pp. 431–39.

Pudelko M, Tenzer H, and Harzing A (2015) Cross-cultural management and language studies within international business research: past and present paradigms and suggestions for future research. In: Holden N, Michailova S and Tietze S (eds) *The Routledge Companion to Cross-Cultural Management*. London/New York: Routledge, pp. 85–94.

Romani L (2008) *Relating to the Other: Paradigm Interplay for Cross-Cultural Management Research*. Saarbrücken: LAP.

Romani L and Primecz H (2019) Promoting and demystifying paradigm interplay: reflexive practices on a study of Turkish mobile professionals. *Studi di Sociologia* 57(1): 31–44.

Romani L, Barmeyer C, Primecz H, et al. (2018a) Cross-cultural management studies: state of the field in the four research paradigms. *International Studies of Management & Organization* 48(3): 247–63.

Romani L, Mahadevan J, and Primecz H (2018b) Critical cross-cultural management: outline and emerging contributions. *International Studies of Management & Organization* 48(4): 403–18.

Romani L, Primecz H, and Topçu K (2011a) Paradigm interplay for theory development: a methodological example with the Kulturstandard method. *Organizational Research Methods* 14(3): 432–55.

Romani L, Sackmann SA, and Primecz H (2011b) Culture and negotiated meanings: the value of considering meaning systems and power imbalance for cross-cultural management. In: Primecz H, Romani L and Sackmann S (eds): *Cross-Cultural Management in Practice. Culture and Negotiated Meaning*. Cheltenham: Edward Elgar, pp. 1–17.

Sackmann SA and Phillips ME (2004) Contextual influences on culture research: shifting assumptions for new workplace realities. *International Journal of Cross Cultural Management* 4(3): 370–90.

Schultz M and Hatch M (1996) Living with multiple paradigms: The case of paradigm interplay in organizational culture studies. *The Academy of Management Review* 21(2): 529–57.

Segal JP (2009) *Efficaces ensemble – un défi français*. Paris: Seuil.

Simmel G (1908) *Soziologie. Untersuchungen über die Form der Vergesellschaftung*. Berlin: Duncker & Humblot.

Spencer-Oatey H and Franklin P (2009) *Intercultural Interaction. A Multidisciplinary Approach to Intercultural Communication*. London: Palgrave Macmillan.

Stahl GK, Miska C, Lee HJ, et al. (2017) The upside of cultural differences: towards a more balanced treatment of culture in cross-cultural management research. *Cross Cultural & Strategic Management* 24(1): 2–12.

Thomas A (2010) Culture and Cultural Standards. In: Thomas A, Kinast EU, and Schroll-Machl S (eds) *Handbook of Intercultural Communication and Cooperation. Basics and Areas of Application*. Göttingen: Vandenhoeck & Ruprecht, pp. 17–27.

Thomas A (2018) Orientation in cultural and ethnic diversity. The concept of cultural standards. In: Thomas A (ed) *Cultural and Ethnic Diversity. How European Psychologists Can Meet the Challenges*. Göttingen: Hogrefe, pp. 25–37.

Ybema S and Byun H (2009) Cultivating cultural differences in asymmetric power relations. *International Journal of Cross Cultural Management* 9(3): 339–58.

Zølner M (2019) Local intermediaries and their organisational identification in a French subsidiary. *European Journal of International Management* 13(1): 88–110.

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RESEARCH ARTICLE

A Multi-Paradigm Modeling Framework to Simulate Dynamic Reciprocity in a Bioreactor

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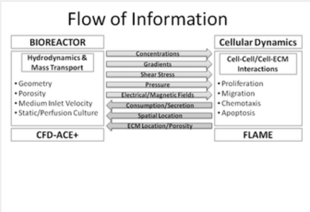
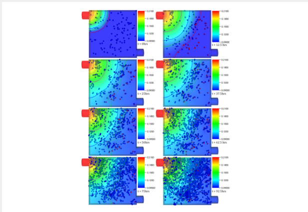
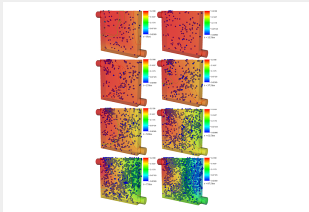
Abstract

Despite numerous technology advances, bioreactors are still mostly utilized as functional black-boxes where trial and error eventually leads to the desirable cellular outcome. Investigators have applied various computational approaches to understand the impact the internal dynamics of such devices has on overall cell growth, but such models cannot provide a comprehensive perspective regarding the system dynamics, due to limitations inherent to the underlying approaches. In this study, a novel multi-paradigm modeling platform capable of simulating the dynamic bidirectional relationship between cells and their microenvironment is presented. Designing the modeling platform entailed combining and coupling fully an agent-based modeling platform with a transport phenomena computational modeling framework. To demonstrate capability, the platform was used to study the impact of bioreactor parameters on the overall cell population behavior and vice versa. In order to achieve this, virtual bioreactors were constructed and seeded. The virtual cells, guided by a set of rules involving the simulated mass transport inside the bioreactor, as well as cell-related probabilistic parameters, were capable of displaying an array of behaviors such as proliferation, migration, chemotaxis and apoptosis. In this way the platform was shown to capture not only the impact of bioreactor transport processes on cellular behavior but also the influence that cellular activity wields on that very same local mass transport, thereby influencing overall cell growth. The platform was validated by simulating cellular chemotaxis in a virtual direct visualization chamber and comparing the simulation with its experimental analogue. The results presented in this paper are in agreement with published models of similar flavor. The modeling platform can be used as a concept selection tool to optimize bioreactor design specifications.

Figures







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Introduction

The diseases of *cellular deficiency* [1] can be only treated if the lost cell population is either regenerated or compensated using autologous substitutes [2], [3]. Given that certain adult human tissues lose their capacity to regenerate [4], they rely exclusively, in case of a critical injury, on functionally similar substitutes [4]–[7]. The principles of tissue engineering can be used to develop such biological substitutes, with remarkably similar properties as those of the host tissues, *in vitro* [4], [6]–[9]. This requires recapitulation of certain key developmental events *ex vivo* thereby necessitating tight control over the artificial growth environment [3], [7], [10]. Bioreactors, which have evolved significantly in both their complexity and functionality over the last two decades, are devices that have been successfully utilized towards this end [2], [3], [10]. Apart from their primary design objective (which is to regulate the cellular microenvironment to support cell viability, promote their 3D organization and provide the cells with spatiotemporally controlled signals) they also offer the user the possibility to seed cells dynamically within 3D matrices, overcome the constraints inherent to static cultures and stimulate the developing constructs physically [3], [10].

Despite the technological advances that have been made in the sector of regenerative medicine and bioreactor technology, there is still a pressing need for safe and clinically efficacious autologous substitutes [3]. Translating regenerative medicine from bench to bed-side would not only require a good product but also robust, controllable and cost-effective manufacturing bioprocesses that are compliant with the evolving regulatory frameworks [3], [11]. Bioreactors serve ideally towards this end as they are the key element for the development of automated, standardized, traceable, cost-effective and safe manufacturing processes for engineered tissues for clinical applications [3].

However, utilized primarily as black boxes, where trial and error eventually leads to the desirable cellular outcome [3], [12], bioreactors have an enormous ground to cover for that eventuality to be realized. Currently, the yields are qualitatively poor and the process of cell growth is often not reproducible. The problem stems from the fact that little is known about the impact of specific bioreactor mass transport characteristics and features on the expansion and growth of cells within the device. Investigators in recent years have begun applying computational tools [12], [13] to study mass transport inside the bioreactor and how that may influence cell dynamics, but this extremely complex interplay has thus far proven elusive.

Analyses based on tackling directly the differential equations governing transport have not only been successful in quantifying mass transport and hydrodynamics inside the bioreactors; their use has been extended to, given certain assumptions, studying cellular dynamics as well [12], [14]. Such models usually either assume absence of neo-tissue within the interconnected pore space in a scaffold or cell attachment only along the surfaces of the scaffold [12]. The differential approach models the cell population, the surrounding extra-cellular framework and nutrients as distributed continua [14]. The matrix in which the cells grow can be treated as a porous medium [14] and one can utilize a wide variety of available computational methods to quantify the distribution of any number of substances being transported and diffusing inside it. Whereas the continuum approach captures the transport phenomena quite accurately, the fact that it investigates biological phenomena at cell *population* level, disregarding entirely the cellular heterogeneity – central to biological function [14], [15] – and the low-level system details [16], hinders detailed analysis of cellular dynamics [11], [17], [18].

In order to understand the impact of cell level behavior on the overall cell population discrete models can be employed [14]–[16], [18]. The cellular automata approach has been used extensively to trace the microscopic details of cellular dynamics more directly and accurately by attributing a set of evolution/transition rules to the computational grids that can represent biological entities such as the cell or the physical microenvironment [14], [19]. The models that have been tried using this approach usually assume a constant supply of nutrients, which is not fully reflective of the actual conditions even under carefully designed experiments [15], [20]. Furthermore, the discrete models available in the literature, despite capturing processes such as contact inhibition, persistent random walk and cell division with marked accuracy, do not consider the impact of chemotaxis and apoptosis on the overall growth dynamics of a cellular colony [15], [20]. More recently, hybrid models, which are a combination of the continuum and discrete approaches, have been utilized to study the impact of transport phenomena on cellular dynamics [14], [16], [21], [22]. Despite being a significant advancement over both the continuum and discrete approach, most of the limitations of the cellular automata models apply to the hybrid models as well. Additionally, the fact that these models are computation- and time-consuming makes it difficult for them to be considered for three-dimensional systems.

Before exploring the relevant hybrid models it needs stating that the hybrid approach itself is not novel and has been applied to simulate a variety of non-biological phenomena. Examples include coupled finite element-flux corrected transport method/finite volume approach to predict electrostatic fields, electrohydrodynamic flow, particle charging and turbulent motion, and their mutual interaction in 3D models of a single wire-plate electrostatic precipitator [23]; finite-element/finite-volume approach to model flow and transport in heterogeneous porous media [24]; computational-fluid-dynamics (CFD)/agent-based modeling (ABM) approach to simulate a gas turbine engine [25]; finite-difference/finite-element approach to model temperature increase in biological vascularized tissues produced by radio-frequency exposure [26]; and discrete element method/compartment modeling to analyze granular mixing [27] amongst others. Furthermore, attempts have been made to study gas-liquid flow in bubble column reactors [28] and gas-liquid-solid three phase flow using a Lagrangian-Eulerian approach [29], [30].

Chung et al (2006) [5] developed a mathematical model to explain tissue growth inside a scaffold by treating the cell-scaffold construct as a porous medium, also incorporating cell diffusion to account for cell random walks. Galban and Locke (1999a, 1999b) [31], [32] adopted a similar approach and utilized species continuity equations and the volume average method to model *in vitro* growth of cartilage tissues. Both these modeling efforts produced interesting results and valuable insight – within the limitations of continuum models of course. Lemon and King (2006) [33] utilized a multiphase model to capture the growth of biological tissue inside a rigid scaffold. The model, based on the mixture theory where each tissue component – cells, water and a solid scaffold material – was treated as a continuum on the macroscale, accounted for cell division as well as apoptosis. Although it dealt very elegantly with the mechanical aspects of the system, necrosis was not considered in the model. Moreover, mitosis was considered to be proportional to the volume fraction of nutrients, cells and water; whereas apoptosis was considered to be proportional to the volume fraction of cells – thereby disregarding the dependence of such behavior on cellular and spatial heterogeneity. Similarly, Flaibani et al (2010) [34] modeled the spatiotemporal evolution of cell heterogeneity in a porous scaffold by solving the relevant PDEs, (discretised using the finite volume approach). The model considered perfusion conditions. These models can capture the population level behavior quite adequately, yet involve assumptions that lead to ignoring of important behavior such as cell migration, apoptosis, necrosis, chemotaxis, variations in the spatiotemporal microenvironment. Thus, a comprehensive picture of the synergistic dynamic interplay that exists in biological as well as tissue engineering systems remains a challenge.

On the other hand, Cheng et al (2006) [15] used the discrete approach to model the dynamic process of tissue growth in a 3D environment. Their model was an improvement over a 2D model developed by Lee et al (1995) [20]. The model considered a population of cells executing persistent random walks on the computational grids, cell-cell collisions and proliferation until confluence. The model assumed constant nutrient and growth factor concentration in space and time and did not consider cell death (apoptosis or necrosis) and chemotaxis. In a more recent model, Cheng et al (2009) [16] utilized the continuum-discrete approach to model the complex interplay that exists between cell populations and mass transport dynamics. Cell interactions were modeled using the discrete CA approach whereas diffusion and consumption of nutrients were based on a transient PDE approach. The dependence of cell division and cell migration on nutrient concentration, which is not to be confused with chemotaxis, was also accounted for. As migration speed was proportional to nutrient concentration, lower nutrient concentration meant lower migration speed. Although the latest model presented by Cheng et al (2009) [16] remains one of the most complete in the literature, it too did not consider chemotaxis and necrosis. Galbusera et al (2008) [22] adopted a similar strategy to create a software framework for computational modeling of tissue engineering experiments. Cell population in this framework is modeled using the 'discrete cells in a continuum space' (Galbusera et al., 2008) approach [22]. The finite element approach was used to model the cell environment. The group presents a 3D microscopic model but only a 2D macroscopic model. Michaelis-Menten kinetics were used to calculate oxygen consumption by the cells (which makes oxygen consumption a population behavior). Furthermore, the model considers necrosis, due to lack of oxygen, occurring when the oxygen concentration falls to less than 50% of the initial value. The model did not consider chemotaxis.

Despite their focus on microorganisms, hybrid models developed by Lapin et al deserve a mention due to the ease of extension of the models to animal cells. Lapin et al modeled microorganism population behavior in bioreactors by opting for an individual-based approach [35]–[37] whereby the dynamic behavior of the system as a whole can be traced to the behavior of individual organisms. Their initial model [35], [37] focused on simulating temporal and spatial behavior of a population of oscillating yeast cells based on glucose concentration fields in a bioreactor. In order to achieve this, computational fluid dynamics (CFD) – modeling the turbulent flow fields in the bioreactor – was coupled with Eulerian-Lagrangian representation of the system, where the extracellular environment was based on the Euler approach and the distributed biophase was characterized by a discrete cell ensemble (Lagrange) approach. The model considers cell migration by superimposing random movement due to turbulent dispersion on the convective flow. The cell in this instance, however, does not mean a 'real' living cell, rather a computational element that represents a large collective of real cells. In its advanced form [36], [37] the model was extended to simulate E. coli population dynamics in a stirred-tank bioreactor with non-ideal mixing. In particular, Lapin et al modeled glucose uptake by the bacteria, which depends on a combination of the extracellular glucose as well as intracellular metabolite concentrations. The investigators observed distinct differences in cell viability at various scales of operation. The novelty of the model lies in its strategy to trace population behavior by considering the individual cell response as a result of key reactions of the central metabolism, which we feel is a more mature, if computationally expensive, way of approaching biological complexity. Certain assumptions of this model are worth highlighting here: firstly, the Lagrangian representation of the model is pseudo-discrete. Each computational element represents a population of physical cells. It can be argued that this makes the simulation computationally economical but has the disadvantage of ignoring various individual-level details. Furthermore, like others previously discussed, the models do not consider proliferation, chemotaxis, or apoptosis – features particularly important in tissue engineering bioreactors (the focus of our work).

A modeling approach that has been gaining interest amongst biologists and mathematicians alike is the agent-based modeling (ABM). Drawing on different fields such as computer science, artificial intelligence, complex systems, and the social sciences [18], [19], [38]; ABM belongs to a class of discrete mathematical approaches in which a system is modeled as a collection of autonomous decision making entities that possess the capacity to detect local information and act at each of several discrete *time steps* based on a set of logical and/or mathematical rules attributed to them [19], [39]. Although quite similar in flavor to the cellular automata (CA) approach, ABM differs from CA in that ABM employs mobile agents, is characterized by asynchronous agent behavior – i.e. allowing agents to update their states independently of each other – and allows the user to incorporate stochastic elements in the rule-set attributed to the agents [19]. Furthermore, the CA approach, which can be described as a fixed grid of interacting finite-state machines, lacks internal memory, which leads to a combinatorial explosion of stages when considering even trivial communication [17]. As a result, when it comes down to representing complex systems, the agent-based approach appears to offer certain advantages over the cellular automata approach.

A design tool capable of predicting the impact a bioreactor's design specifications, such as its flow-rate, inlet/outlet position, geometry, and a given cell's biological properties, such as its nutrient consumption or metabolic rate, can have on the growth (and differentiation) dynamics of the overall cell population will therefore not only be immensely helpful in optimizing bioreactor design and construction, but may help uncover the governing dynamics that regulate development. In this study a multi-paradigm 'transport-agent' model, capable of predicting, based on a set of logical, algebraic, stochastic and differential rules, the impact of bioreactor mass transport and hydrodynamics on the growth dynamics of cells in a virtual bioreactor is presented. The novelty of the platform is that in addition to capturing cell dynamics as a result of interactions between individual cells (a feat previously achieved by published CA and agent-based models), it also considers the impact that local transport has on the cells and how the cells might be able to indirectly alter their local environment due to behavior like cell division, cell aggregation or extra-cellular matrix synthesis or digestion. The platform can therefore capture *dynamic reciprocity* [40], [41]; an emergent phenomenon.

To achieve this, we have pursued the tight coupling of two mature modeling platforms; first, the Flexible Large-scale Agent Modeling Framework (FLAME) [17], [42]–[45], an agent-based system, with a computational multi-physics transport phenomena platform (CFD-ACE+, ESI Group, Paris, France). FLAME captures the rules that govern cell growth and proliferation whereas CFD-ACE+ is employed to simulate bioreactor hydrodynamics, mass transport processes and other biomechanical effects (for example, shear or strain triggered cellular responses). The platform considers cellular behavior in 3D. Through the platform we wanted to test the hypothesis that bioreactor geometries, bioreactor variables and initial conditions are crucial to cell development and that the integrated framework could be used to capture that and optimize bioreactor design. In this paper, various bioreactor variables are tested virtually. The results of the *in virtuo* experiment deploying the integrated model are presented and discussed. The bioreactor models considered were relatively simple, although the platform has the capability to deal with geometries, perfusion/stimuli characteristics and cellular populations of arbitrary complexity.

Methods

Quantifying cell population dynamics as well as the biophysicochemical microenvironment are the important aspects of modeling tissue engineering systems [22]. As discussed above, the impact of spatial and cell-population heterogeneity can be best modeled using the discrete approach whereas the continuum approach remains the most accurate way of capturing the bulk phenomena. The modeling platform was therefore composed of two integrated and communicating elements that can simulate the various biological processes which work synergistically to produce behavior of staggering complexity. A brief description of each of the two components is therefore essential.

2.1 Agent-Based Modelling

When the number of individuals to be modeled in a process is relatively small (roughly 10^5–10^6), emergent phenomena are the primary interest and spatial considerations are important (as individual entities can be localized in space), an agent-based approach can be utilized [43]. As defined by Wooldridge [46], "*an agent is an encapsulated computer system that is situated in some environment and that is capable of flexible, autonomous action in that environment in order to meet its design objectives*". Therefore, by definition, an agent possesses well defined boundaries, has the ability to sense its environment and act on its environment, can control its internal state as well as behavior, have particular goals to achieve, can act in the anticipation of future goals, and respond in timely fashion to changes that affect its environment [46]: features that in principle make an agent very similar to a cell.

The agent-based approach decomposes the problem in terms of autonomous entities. These autonomous entities engage in flexible, high-level interactions, a feature that attributes to the system multiple loci of control. Decision-making is therefore limited to the agents' actual situation as opposed to some external entity's perception of this situation [46]. The fact that agent interactions are flexible allows the user to attribute to the components the ability to make decisions about the nature and scope of their interactions at run-time, thereby bypassing the need to specify every possible inter-agent link (an impossibility given the nature of any biological system's complexity) [46].

The agent-based paradigm possesses structures that can represent and manage organizational relationships, such as roles, norms and social laws [46]. Furthermore, the presence of interaction protocols (to form new groupings and disband unwanted ones) [46] coupled with the ease with which collectives, such as teams, could be modeled enables the agent-oriented mind-set to provide suitable abstractions [46] necessary to model complex, especially biological, systems. And finally, the fact that ABM can conduct an organizational updating [46] during run time (in case an agent is destroyed) makes the agent-based philosophy more suitable to address the dynamic nature of biological systems.

Chavali et al (2008) [19] listed desirable framework capabilities that are important to address key challenges in immunology. They can be extended to frameworks that are being developed to capture cellular behavior. Such frameworks must simulate non-linear and dynamic behavior, cell-cell and cell-environment interactions and cell population behavior as a function of population heterogeneity; attribute the cells with features such as memory (to keep track of various prior interactions) and adaptability (based on the external environment); and permit visualization of the resulting phenomena that emerges from the combined interactions between the cells considered in the model [19]. An agent-based method, in particular the Flexible Large-scale Agent-based Modeling Environment (FLAME), provides the investigator the ability to do precisely that.

Moreover, FLAME allows simulation of large numbers of agents to be run on parallel computers [17], [42]. The platform was developed at the University of Sheffield for the *Epitheliome* project and has been used to model the emergent behavior of biological as well as economic systems [18], [42]. The FLAME framework, which enables creation of agent-based models that can be run on high-performance computers, is based on the logical communicating extended finite state machine (X-machine) theory [17], [47]. Agents are modeled as communicating stream X-machines, an attribute that allows them to interact with each other. This modeling mechanism provides a sensible way of dealing with problems associated with state explosion, which afflict many efforts at modeling complex biological systems [17], [43], [45]. Furthermore, being inherently hierarchical, an X-machine is able to link different modeling paradigms; an attribute that is critical to the success of this platform [43]. For more information on FLAME, the interested reader is directed to http://www.flame.ac.uk/.

2.2 Transport Phenomena

The hydrodynamics inside the bioreactor as well as the mass transport were quantified by solving the governing transport equations (i.e., conservation of mass, momentum and species) using the finite-volume method. In this methodology, the computational domain is divided into a set of control volumes (CVs) by means of a grid. The finite volume method, by using the integral form of the general transport equation, preserves its conservative nature. The generalized transport equation for a conserved quantity Φ is shown below as equation 1. This equation, by appropriately assigning parameters and source terms, effectively accounts for the conservation of mass, momentum, species and reaction of species. In the equation *ρ* is the fluid density and *U* the velocity vector. On the left hand side of the equation: the first term accounts for the transient nature of the process, the second for convection and the third for diffusive processes. The term on the right hand of the equation, a generalized source term, accounts for variable-specific mechanisms; such as the pressure gradient in the momentum equation manifestation of the general transport equation, or the chemical reaction as far as the species conservative equation is concerned, or the secretion or consumption of a molecule by the cells, when continuity is considered.

$$\frac{\partial}{\partial t}(\rho\Phi)+\nabla.(\rho U\Phi)-\nabla.(\Gamma_{\Phi}\nabla\Phi)=S_{\Phi}$$

(1)

Equation 1 was solved in its full transient form. As a suitable abstraction, oxygen was assumed to be the limiting scalar, although the platform can consider multiple scalars and, if necessary, can capture any reactions that may exist between these scalars. Consumption of oxygen was modeled by representing the cells, or more appropriately the agents, as proliferating sinks – covered by the term on the right in equation 1. It must be noted here that this equation is easily extended, in a Darcian sense, to account for porous media, by incorporating local porosity and permeability terms (i.e. local void fractions and resistances) at every computational cell.

Converting the integral of (1) over the CV into a surface integral yields equation (2), where S represents any of the faces on the CV, whereas $\mathbf{n}_S$ is the unit vector normal to that surface. The convective and diffusive terms are determined using suitable second order accurate interpolation schemes [48].

$$\int_{CV}\frac{\partial}{\partial t}(\rho\Phi)dV+\sum_{faces}^{surface}\int_{S}[\rho U\Phi-\Gamma_{\Phi}\nabla\Phi].n_{s}dS=\int_{V}S_{\Phi}$$

(2)

Pressure and velocity fields were coupled using the SIMPLEC algorithm [49] and an *algebraic multigrid* (AGM) solver was employed [50] as the iterative equation solver. The AGM solver uses a hierarchy of grids, from fine to coarse, and back to fine, to solve the resulting set of pseudo-linear equations: After obtaining the residual on the fine grid, iterations are performed on the coarse grid to obtain corrections (imposing fine-grid residual as the source term). The AGM solver works by interpolating the corrections to the fine-grid and updating the fine grid solution, and repeating the entire procedure until the residual is reduced to the desired level. This way, errors of multiple wavelengths are improved upon simultaneously.

The numerical procedures described above were implemented in CFD-ACE+ in this study. This is a multi-physics proprietary computational tool that allows easily the interfacing with external modules, thus incorporating additional physics (for example, the effect of electrical or magnetic fields, temperature or deformable substrates on cells). Integrating FLAME with CFD-ACE+ provides an efficient multi-paradigm modeling framework that was used to set up a multi-scale model displaying cellular dynamics inside a virtual bioreactor. Figure 1 shows the exchange of information between the agent-based model and the transport model that is at the heart of the platform presented in this paper.

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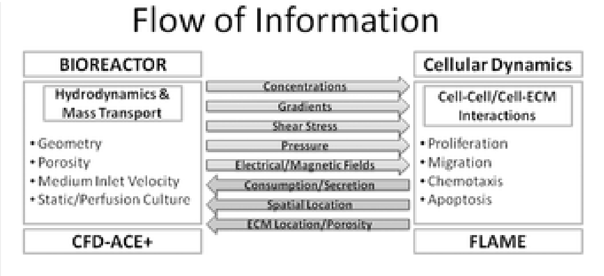

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Figure 1. Flow of Information in the modeling framework.

The figure shows the communication between the transport-phenomena and agent-based modules that is at the heart of the modeling platform. Information relevant to bioreactor hydrodynamics and mass transport is communicated from the transport-phenomena module to the agent-based module where cells, modeled as agents, detect the local concentrations (and other continuum variables) and act based on the rules attributed to them. The cellular information is then relayed back to the transport-phenomena module to complete the circuit.

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2.3 Model Features

2.3.1 oxygen transport and consumption.

The cells were assumed to be seeded in a porous scaffold inside a bioreactor and were supported by the influx of oxygenated medium. Two virtual bioreactors, enclosing a porous scaffold, of different geometries but same volume were constructed. The two bioreactor geometries can be seen in Figures 2, 3 (geometry A) and 4, 5 (geometry B), and the dimensions of the bioreactors are listed in Table 1. Bioreactor construction was followed by a grid independence analysis, which was conducted on one of the bioreactors (geometry A). The bioreactor was assigned structured (50,000; 100,000; 200,000 and 400,000 elements) as well as unstructured (100,000 and 400,000 elements) grids. The results indicated no appreciable difference between a bioreactor with a 100,000 element structured grid and a bioreactor with a 400,000 element unstructured grid. As a result, to strike a balance between result accuracy and computational time, the bioreactors were solved using 100,000 elements structured grids. Furthermore, the scaffolds were assigned constant isotropic porosity and permeability (75% and 10^{-10} m^2 respectively) and tested for medium inlet velocities of 0.01 m/s and 0.001 m/s. Please refer to Table 2 for a description of different test cases.

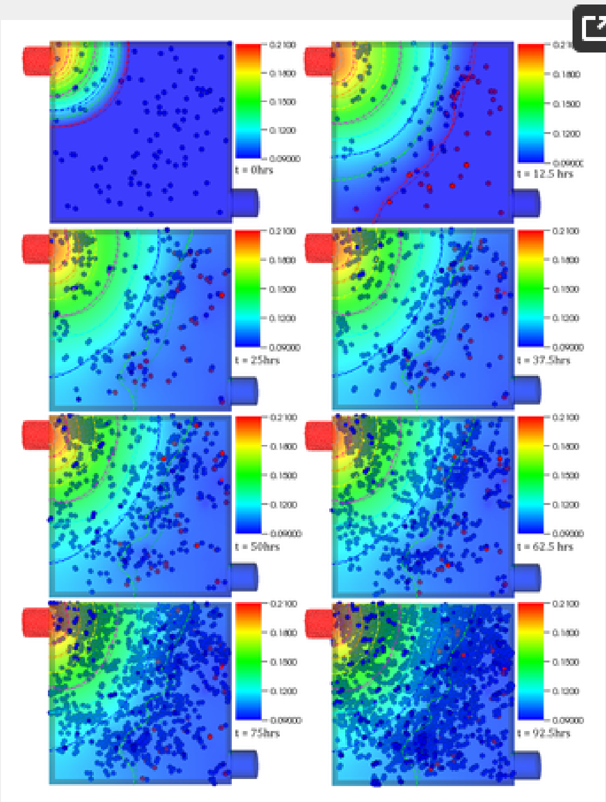

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Figure 2. Case 1 results.

Temporal evolution of cell population and nutrient concentration inside a 3D scaffold bioreactor (geometry A) with a medium inlet velocity of 0.001 m/s. The top-left port on the bioreactor serves as the inlet whereas the bottom-right port serves as the outlet. The final frame captures cell distribution at the end of 4 (physical) days – the time interval between snapshots (left to right) is 12.5 hours. The initial cell density was 100.

https://doi.org/10.1371/journal.pone.0059671.g002

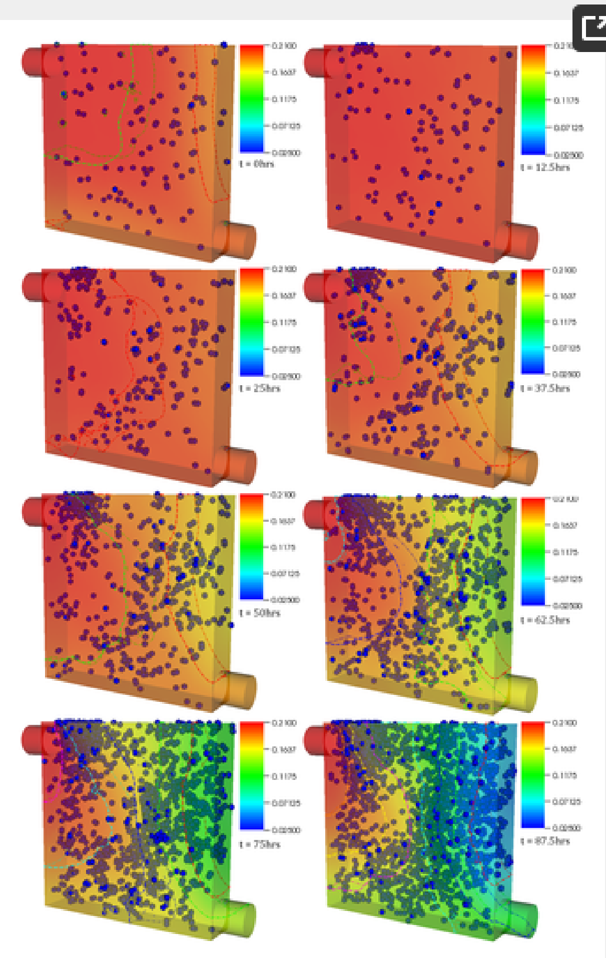

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Figure 3. Case 2 results.

Temporal evolution of cell population and nutrient concentration inside a bioreactor (geometry A) with a medium inlet velocity of 0.01 m/s. The final frame captures cell distribution at the end of 4 (physical) days – the time interval between snapshots (left to right) is 12.5 hours. The initial cell density was 100. The concentration contours can be observed to change continuously throughout the simulation. This is in contrast with physical systems with no cells inside where such behavior would not be possible after the flow becomes stationary beyond initial transients. This demonstrates the platform's ability capture dynamic reciprocity.

https://doi.org/10.1371/journal.pone.0059671.g003

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Bioreactor Variables		
Geometries	2	
Scalar	Oxygen	
Initial Concentration[14]	$0.21\ mol\ m^{-3}$	
Scalar Diffusivity in the Media[14]	$10^{-5}\ m^2/h$	
Scaffold Porosity	75%	
Scaffold Permeability	$10^{-10}\ m^2$	
Medium Density	$1000\ kg/m^3$	
Medium Viscosity	0.001 kg/m-s	
Medium Inlet Velocity	0.001 m/s, 0.01 m/s	
Bioreactor Dimensions	Length	1 mm
	Width	1 mm
	Depth	0.2 mm

The table lists various volume, boundary, and initial conditions applied to compute mass transport inside the bioreactors. The dynamic relationship between cell proliferation and mass transport of oxygen was investigated in two bioreactors of same volume but different geometries (shown in figures 2 and 4). Oxygenated medium was introduced at two different velocities: 0.001 m/s and 0.01 m/s.

doi:10.1371/journal.pone.0059671.t001

Table 1. Bioreactor Variables.

https://doi.org/10.1371/journal.pone.0059671.t001

Case	Bioreactor Geometry	Initial Cell Density	Medium Inlet Velocity (m/s)	Flow Rate (L/s)	Relevant Figures/Videos
Case 1	A	100	0.001	0.02	Fig 2/S2
Case 2	A	100	0.01	0.2	Fig 3/S3
Case 3	B	5	0.001	0.002	Fig 4/Fig 5/S4
Case 4	B	5	0.01	0.02	Fig 5/S5

The table lists various test cases simulated for the purposes of this investigation and relevant parameters, such as medium flow rate, and relevant figures and supplementary material.

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Table 2. Test Cases.

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Concentration gradient of oxygen is known to affect tissue-growth rate in bio-artificial scaffolds [16]. Therefore, the model was designed to study cell growth in a continuous medium perfusion system with oxygen being the limiting nutrient. After the bioreactor-scaffold complex was suffused with virtual cells, oxygenated medium was pumped in at the velocities (and corresponding flow rates) listed in Table 2. Oxygen transport inside the bioreactor occurred by convective as well as diffusive processes. The diffusivity of oxygen in the medium was taken as $10^{-5}\ m^2/hr$ [14]. The medium supplied to the bioreactors was assumed to be carrying oxygen at a concentration of $0.21\ mol/m^3$ [14]. Oxygen consumption was modeled using cells as proliferating and migrating non-zero sinks consuming oxygen at $3.39\ mol\ kg\ m^{-3}\ s^{-1}$ [14]. In the agent-based component this amounts to oxygen consumption by each cell at a rate of $12.2\ mol\ m^{-3}\ hr^{-1}$.

Oxygen (or any other substance) consumption (or secretion), modeled as an individual-level event, was accounted by the source term represented as S_Φ in (1). The equation was implemented as migrating non-zero sinks. Generally speaking, the source term can be represented by equation 3, which displays the dependence of S_Φ on existing scalar concentration.

$$S_\Phi = S_c + S_p \Phi_p \tag{3}$$

Equation 3 involves a constant as well as a linear dependence of the source term on scalar concentration. In cases where the relationship is non-linear, it must be linearized [51]. Equation 3 was applied to control volumes with cells in them (as derived from the agent-based module of the platform) and with appropriate summations in the case of multiple cells within a single control volume.

Oxygen concentration in this model is assumed to vary based on the bioreactor hydrodynamics, mass transport and cell proliferation. Dirichlet and Neumann boundary conditions were applied as needed. Oxygen transport and consumption, in sync with cellular proliferation and migration, was calculated for periods of four to six days depending on the case and the fate of the cells in the virtual bioreactors.

2.3.2 Cell population dynamics.

The platform is designed to incorporate a variety of behaviors displayed by cells: migration, proliferation, differentiation, chemotaxis, apoptosis, necrosis and other processes as needed. The agent-based component considers each virtual cell to be an agent governed by a set of logic rules that is capable of displaying migration, proliferation, chemotaxis and apoptosis. Differentiation was not considered in the cases tested in this paper. The biological rules governing the virtual cells, listed in Table 3, are controlled by constants, for example cell cycle, as well as variables – which in turn emerge from the transport phenomena component – such as oxygen concentration gradients. The cells were assumed to be non-deformable spheres of radius 10 μm each and capable of consuming oxygen at a rate of 12.2 mol $m^{-3}hr^{-1}cell^{-1}$ when available. Initial cell placement inside the bioreactor-scaffold complex was random.

Cellular Variables	
Persistence Time[14–16, 20, 53]	2 hours
Post Collision, pre-Division Stationary Phase[20]	1 hour
Cell Cycle & Division Probability of Cell Population[53]	18 hours (64%)
	24 hours (32%)
	32 hours (4%)
Maximum Random Speed	10 μm/hr
Cell speed during Chemotaxis	20 μm/hr
Oxygen Consumption Rate[14]	3.39 mol kg m^{-3} s^{-1}
Chemotaxis Ensues at Scalar Concentration[52]	0.0672 mol m^{-3}
Hypoxia-induced Apoptosis	15 hours
Cell Density in Bioreactors	100, 5

The table lists parameters pertinent to the cells as well as rules the cells followed during the computation. For example, under normoxic condition cells displayed persistent random walk changing direction once every two hours. Cells would only stop if it is in contact with another cell or about to undergo mitosis. Furthermore, chemotaxis ensues if a cell experiences local oxygen concentration of less than 0.0672 mol m^{-3}. Failure to move to a normoxic region within 15 hours since the inception of chemotaxis leads to hypoxia-induced apoptosis.
doi:10.1371/journal.pone.0059671.t003

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Table 3. Cellular Variables and Rules.
https://doi.org/10.1371/journal.pone.0059671.t003

The cells could migrate by choosing either a persistent random walk or chemotaxis. The cells displayed persistent random walk [15], [16], [20] if the local oxygen concentration >0.0672 mol/m^3. If, however, the local oxygen concentration dropped below 0.0672 mol/m^3, the cells began to display chemotaxis in a bid to move to an oxygen-rich region. This value is equal to 0.3% of the initial oxygen concentration, and was decided upon after reviewing the work of Liu et al (2007) [52] who reported induction of hypoxia at oxygen concentration of 0.3% in HCT 116 colon carcinoma cells. The cells were assumed to divide until confluence or until the point where there was not enough oxygen available to them. Confluence, or the point where the bioreactor is completely filled with cells, was achieved when each cell was bonded to at least four other cells. The cells divided based on a division probability assigned to them: 64% of the cells divided by eighteen hours, 32% by twenty four hours and the remaining 4% by thirty hours [53]. The daughter cell is positioned at a random orientation relating to the coordinates of the parent cell, and in the immediate vicinity of the parent cell.

Another advancement this platform has to offer is that it takes into account cell apoptosis that may occur due to cells experiencing hypoxia in oxygen deficient areas created in the bioreactor due to cell growth or other factors such as low medium inlet rate or deficient mixing. If the local oxygen concentration dropped below 0.0672 mol/m^3, the cells began to express apoptotic proteins. If a cell stayed under the hypoxic condition for more than 15 hours, it died of hypoxia-induced apoptosis. The cells were assumed to exert a repulsive force on each other in case of contact, which was taken from a model developed by Tao et al (2007) [44]. Although the nature of mechanical forces that cells exert on each other is quite complex, the physical forces were resolved using constants instead of variables as our primary objective was to display the platform’s capability to handle such occurrences and to accommodate any such sub-model when available. Please refer to Table 3 for relevant parameters.

2.3.3 Cell migration.

The extracellular environment and cell type affect and dynamically modulate [16] a cell's speed and its persistent time [15], with prostate cancer cells displaying speeds of 8–15 µm/hr in 3D collagen matrices and melanoma cells 20–40 µm/hr in 3D collagen matrices modified with RGD proteins [15], [54], [55]. The scaffold in our case was assumed to have no restraining effect on cell migration. Therefore, despite their presence in a porous scaffold, the cells could move freely in all (three-dimensional) directions. A migration speed was assigned to each cell. As long as the cell displayed persistent random walk, it could acquire a maximum speed of 10 µm/hr. The cell continued moving in a particular direction for two hours after which, based on the availability of space, the cell assumed a new randomly chosen direction, in agreement with [14]–[16], [20], [53]. If, while migrating, a cell came in contact with another cell or the bioreactor boundary, it stopped for an hour, in agreement with [14]–[16], [20], [53], before changing its direction and continuing migrating in a randomly chosen direction. The cells stopped moving prior to dividing and, along with the daughter cell, remained at rest for about an hour after division [20]. While displaying chemotaxis, the speed and direction attributed to the cells were based on the local concentration gradients. Under chemotaxis the cells were assumed to display a set migration speed of 20 µm/hr. If, while performing chemotaxis, a cell ended up in a region rich in oxygen, it went back to displaying the persistent random walk; if not, then the cell moved under the influence of the concentration gradient until it either ended up in an oxygen rich area or it died.

Apoptotic trigger was initiated if the local oxygen concentration dropped below 0.0672 mol/m^3. If a cell remained in an oxygen-deficient region for more than 7 hours, it changed its state (and its color in the visualization platform used to analyze the results of the simulations) indicating that the apoptotic mechanism, physically represented by formation of apoptotic proteins in the cells that lead to cell death, has been triggered. If the cell, in chemotaxis mode at this point, was successfully able to relocate to an oxygen rich region it survived; otherwise if it remained in a hypoxic environment for more than 15 hours since the start of the apoptotic mechanism, it died. The time advancement of the system was organized around computing cycles, usually referred to as *iterations* in agent-based modeling. Since this term has a different meaning in transport phenomena implicit solvers, we shall refrain from using the term – it suffices to say that each computing cycle or iteration was set to 15 minutes and we have found this to be a value that captures the fine features of the system, while leading to reasonable computational time requirements. Table 4 summarizes the rules used in the study.

Behavior	Rule
Proliferation	Cell proliferation occurs until confluence as per assigned probabilities (Table 2)
Migration	Migration occurs either via persistent random walk (under normoxic conditions) or chemotaxis (under hypoxic conditions)
	If local oxygen concentration >0.0672 mol/m^3, cells display persistent random walk
	Cell speed during persistent random walk = 10 µm/hr
	If local oxygen concentration <0.0672 mol/m^3, chemotaxis begins
	Chemotaxis speed = 20 µm/hr
Apoptosis	If a cell experiences hypoxia for more than 15 hours, it dies of hypoxia-induced apoptosis
	If, while performing chemotaxis, a cell ends up in a region rich in oxygen, it goes back to display persistent random walk

The table summarizes the rules used to simulate cellular dynamics.
doi:10.1371/journal.pone.0059671.t004

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Table 4. Rules.
https://doi.org/10.1371/journal.pone.0059671.t004

2.4 Experimental Validation

The ability to capture cellular chemotaxis is a novel feature of the platform. An understanding of the detailed mechanism of chemotaxis finds relevance in, among other sectors, cancer research [56]–[58] and cancer drug design [59]. Typically, the assays utilized to investigate chemotaxis are based on the *two-well* design. Briefly, two wells – one containing a control or buffer substance, and the other the chemoattractant – are connected to each other. Cells are seeded between the wells where they can sense the developing gradient and display an appropriate migration response [60]. Direct visualization assays allow the user to observe cell migration in real-time with the aid of time-lapse microscopy, and are considered the gold standard assay for investigating chemotaxis [60], [61]. Therefore, in order to experimentally validate the platform we simulated cellular chemotaxis in a direct visualization chamber. To achieve this a virtual analogue of the *Insall Chamber* [60] was created. The Insall chamber is a direct visualization chamber developed by *Muinonen-Martin et al* [60] to study chemotaxis using high numerical aperture (NA) oil immersion lenses, which was not possible with other visualization chambers. The Insall chamber consists of an inside well containing the control and an outside well (enclosing the inner well) containing the chemoattractant. The investigators analyzed chemotaxis of MV3 melanoma cells based on linear concentration gradients of Fetal Bovine Serum (FBS). Details regarding the chamber and the experiment can be found here [60].

A virtual Insall chamber was constructed, based on the exact dimensions and specifications of the experimental setup, as obtained directly via private communication [62], [63] with the developers. To ensure consistency between the simulation and experiment, diffusion of FBS was modeled in the half of chamber containing the 0.5 mm bridge as shown in Figure 6. The geometry was discretized using structured grids (approximately 150,000 cells ensured grid independence). The diffusivity of FBS considered in the model was derived from the *Svedberg* [64] equation and calculated to be 8.705×10^{-11} m^2/s. Virtual MV3 melanoma cells were modeled as spheres chemotacting at a speed of 8 μm/hr after sensing a critical FBS concentration (10% of the initial FBS concentration in the outer well). In the absence of the gradient, or in case the local gradient <10% FBS, cells migrated by displaying the persistent random walk. Cellular migration coupled to FBS transport in the virtual *Insall* chamber was modeled for a period of 25 physical hours. As a control, MV3 melanoma cell migration was modeled in the absence of FBS. Statistical significance was determined by conducting paired two-tailed test, where $p<0.05$ was interpreted as significant.

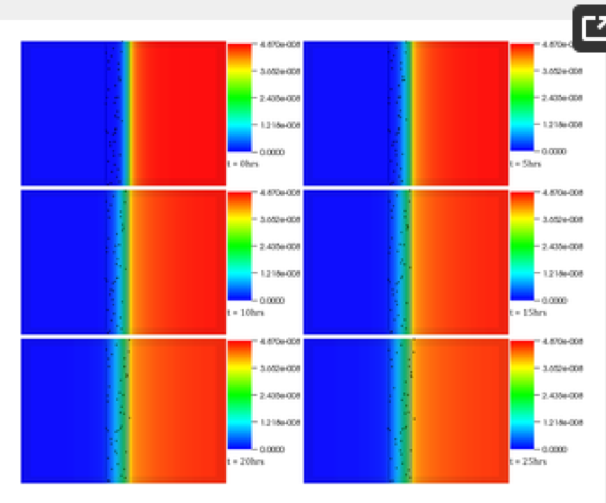

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Figure 6. Experimental Validation of the platform.

The figure shows migration response of MV3 melanoma cells based on FBS concentration gradient. The cells, displaying persistent random walk in the absence of FBS gradient, resort to chemotaxis on sensing FBS concentration. These results, when compared to similarly acquired ones but in the absence of the chemoattractant, confirm the capability of the simulation platform to capture such behaviors. The time interval between snapshots (left to right) is 1 hour. The final frame captures cell distribution at the end of 25 (physical) hours.

https://doi.org/10.1371/journal.pone.0059671.g006

Results

The integrated platform was used to create virtual bioreactors seeded with cells. Figure 2 shows the oxygen concentration contour plot as well as cell distribution inside one of the two different types of bioreactors we tested, at different time instances. The bioreactor is a rectangular prism in shape with two ports: one serving as an inlet (top left) and the other as an outlet (bottom right). Initially, the bioreactor was seeded with one hundred cells. The figures capture the interplay between cell population dynamics and the overall mass transport at various time steps – the final step was recorded at 4 physical days. The migration of cells from the relatively deoxygenated region (bottom right) of the bioreactor to top left can be observed. The dynamic nature of the relationship is best evident by the change in oxygen concentration close to the inlet port – it decreases in intensity in the subsequent time frames, corresponding to a decrease in concentration due to cellular proliferation and resulting increased consumption. Cell division in the region close to the inlet port was initially higher as compared to the rest of the reactor. This propensity of cells to divide closer to the inlet port where oxygen concentration is relatively high is behavior one would normally expect in reality. It must be stressed that this feature was not explicitly coded in the model but, it seems, emerged from the integration of the rule-set with underlying transport phenomena. Widespread proliferation is observed towards the end of the simulation as oxygen concentration exceeds the threshold value throughout the bioreactor. An interesting observation remains the preference the cells show in aligning themselves to the contour curves; thus resulting in an emergent banded distribution pattern – most evident in the second, third and fourth time frames.

Figure 3 shows the temporal evolution of cell population and nutrient concentration in a bioreactor (same as Figure 2) but with a medium inlet velocity (0.01 m/s), an order of magnitude higher than Case 1. As was the case in Figure 2, the cells tend to migrate away from the oxygen deficient region: chemotaxis. The top left region remains an area of high cell division during the initial stages. An important observation is the constant translation of the oxygen concentration contours, which can be better observed in Video S3. It is of interest to note that the banding pattern is significantly less pronounced in this case, and of a different shape than that observed in the previous virtual experiment most probably due to higher oxygen concentration relative to Case I. This behavior merits further investigation as it resonates, albeit modestly, with self-organization observed in biological systems. Questions such as: did lower oxygen availability in Case 1 cause the stressed cells to organize themselves in that manner; if so, can this be extrapolated to other cells, does such behavior lead to more efficient use of resources; what kind of structure would have evolved if cells were assigned more specific rules that govern colony formation, what would be the functionality of such structure; remain a matter of speculation until investigated more rigorously both computationally as well as empirically.

The probable cause behind the emergence of this distribution pattern is connected with the oxygen concentration, and related thresholds. The region close to the curve where patterning is observed is normoxic, whereas the region beyond the curve (closer to the outlet) is hypoxic. As a result cells migrate towards the curve under the influence of the concentration gradient and start behaving randomly as soon as they reach the normoxic region. In effect, the continuous supply of oxygen on one hand and the very random and unpredictable consumption on the other lead to a non-intuitive pattern formation, which spatially does not correspond to where the pure transport solution of the system would place the oxygen threshold iso-contour. Part of this emergent effect comes from the randomness inherent in cell (and agent) migration, but the most significant portion comes from the interplay of these two profoundly different mechanisms that such a hybrid methodology is well-positioned to capture. It must be noted that no matter which threshold is selected (within reasonable and biologically meaningful limits) the pattern formation is persistent in structure (of course varying slightly in exact position and formation) and thus clearly a feature of the coupled system. We found this very interesting and exciting emergent theme in many of the simulations we conducted. Such behavior can be exploited to create multiple mono-layers of defined thicknesses or bi-layers where cells towards the more deprived region of the bioreactor can act as an interface (as in a bone-cartilage hybrid structure).

Figure 4 examines a different bioreactor setup. The top right end of the bioreactor serves as the inlet whereas the entire left as well as bottom ends of the bioreactor serve as the outlet. The medium inlet velocity in this case was 0.001 m/s. The bioreactor was randomly seeded with 5 cells. The simulation was run for a total of 6 physical days. By the second frame (17.5 hours), most of the cells in the deoxygenated region have died – a result of hypoxia-induced apoptosis. The cluster of cells formed by the final frame is a result of the *single* cell that was able to move and begin proliferating in the oxygen rich zone. When the medium inlet velocity was increased to 0.01 m/s (images not shown but supplementary video provided, Video S5), more cells survived which in turn aided in the colonization of the bioreactor. In comparison (Figure 5), the bioreactor with the higher inlet velocity by the final frame ends up with considerably higher number of cells and a distinct growth pattern (resembling the banding arrangement observed in the first case) – once again displaying not only the dynamic nature of the system but the dependence of the spatiotemporal evolution of the system on processes such as chemotaxis and apoptosis. It must be noted that, in some frames, a few cells still appear ‘red’ despite the local oxygen concentration being higher than the threshold. This is not connected with the simulation itself, but it is rather a visualization effect, utilized to highlight the hypoxic **history** of the relevant cells. The cells are no longer hypoxic and continue to grow as any other normoxic cell.

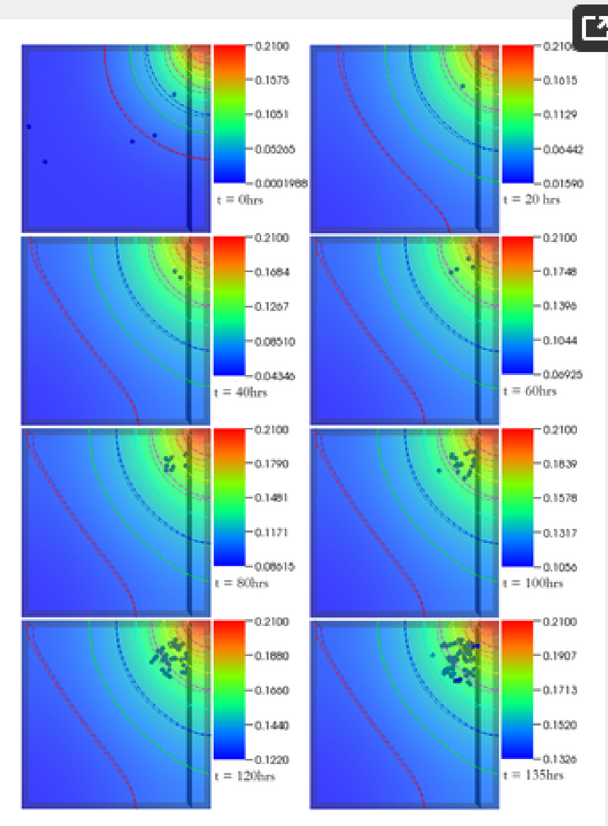

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Figure 4. Case 3 results.

The figure shows temporal evolution of cell population and nutrient concentration inside a bioreactor (geometry B) with a medium inlet velocity of 0.001 m/s. The top right end of the bioreactor serves as the inlet whereas the entire left as well as

bottom ends of the bioreactor serve as outlet. The initial cell density was 5. The time interval between snapshots (left to right) is 20 hours. The final frame captures cell distribution at the end of 6 (physical) days.
https://doi.org/10.1371/journal.pone.0059671.g004

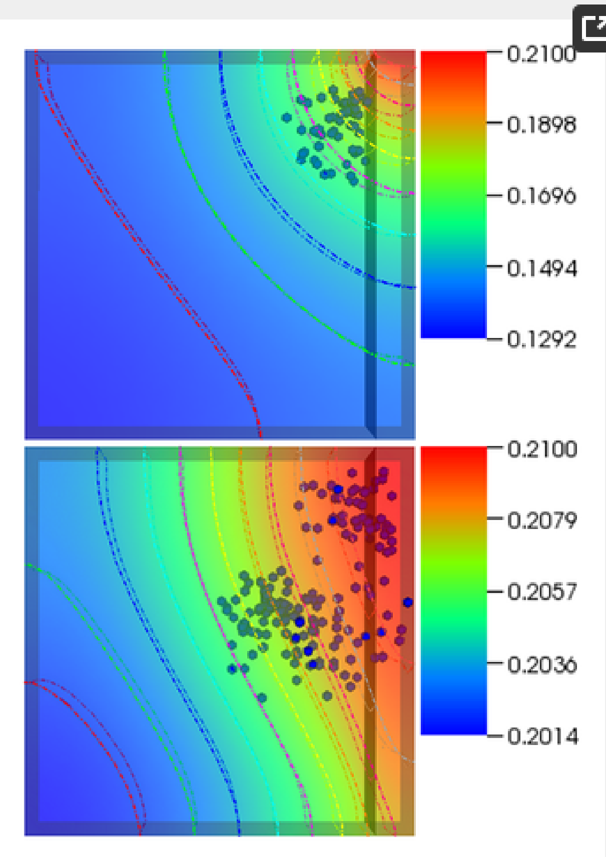

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Figure 5. Different boundary conditions lead to different output.

The figure shows temporal evolution of cell population and nutrient concentration in the same bioreactor set at different medium inlet velocities; 0.001 m/s (top) and 0.01 m/s (bottom). The bioreactor on the right ends up with considerably higher number of cells and a distinct growth pattern. This displays the dynamic nature of the system and the dependence of the spatiotemporal evolution of the system on processes such as chemotaxis and apoptosis. The frames were recorded at 5.5 days.
https://doi.org/10.1371/journal.pone.0059671.g005

Figure 6 shows the evolution of FBS concentration gradient across the bridge and the cells' migration response to the gradient over a period of 25 hours. Cell chemotaxis can be easily observed with the increase in FBS gradient towards the inner chamber. However, few cells that have not committed to chemotaxing can be observed at the end of the simulation on the left hand side of the bridge, but that is because these cells have not yet sensed the critical FBS concentration (10% of the initial concentration in the outer well). Qualitatively, the computational results (refer to Video S6) met expectations and were in very good agreement with the experiment conducted by Muinonen-Martin et al [60], where the melanoma cells were observed to migrate towards the outer well in a comparable manner. A highly significant statistical analysis ($p=1.14\times10^{-69}$), also in agreement with its experimental counterpart, further supported the evidence for gradient directed migration of the MV3 melanoma cells inside the virtual chamber.

The importance of the cellular microenvironment to tissue development was hypothesized as early as 1817 but it took almost a century to confirm this hypothesis when certain regions of amphibian embryos were observed to direct the development of adjacent groups of cells to specific tissue types [41]. *Dynamic reciprocity* [40] takes this behavior a step further and suggests that there exists a dynamic bi-directional relationship between cells and their microenvironment, which is responsible for the overall development of the cellular system. Basically, "*the ECM affects the cell which in turn responds by synthetic and degradative processes causing the composition and the structure of ECM to change which in turn influences the cell and so forth*" [40]. In this paper, we presented a methodology that allows for the rigorous study of this interplay, expanded to include the local transport processes as a part of this synergistic interaction. After all, cellular proliferation *does* affect the local concentration gradients as well as flow profiles, thereby influencing the overall cell growth. In addition to devices such as bioreactors, the amended concept remains applicable to biological systems such as tumor, uterus or compromised tissue. The level of complexity associated with the process makes it quite difficult to be captured by numerical models. The lack of relevant biological data in addition to the complexity of such systems is a reason why comprehensive models for such systems have not been presented yet. However, investigators in the last decade have made significant progress in that direction as discussed in the Introduction.

The modeling platform presented in this manuscript was created keeping bioreactors in mind where the concentration profiles, shear stress and flow profiles etc. influenced initially by the geometry of the bioreactor and later by cellular proliferation play a crucial role in the synthesis of the autologous substitutes required for regenerative medicine. The modeling platform is composed of two working elements: continuum – transport phenomena capturing – and discrete – cellular behavior capturing – elements. Whereas the discrete layer helps the cells to detect the spatial information relevant for processes such as differentiation to occur [65], [66], the continuum layer helps the platform to model the dynamic transport processes that change continuously based on factors such as the number of cells, formation of ECM by the cell colonies or scaffold/ECM degradation. The biggest advantage of the platform, however, remains that it can capture emergent phenomena – a benefit extending from the agent-based side of the platform. As such, the platform can not only help explain non-intuitive observations but has the potential to reveal processes and mechanisms not expected to emerge *a priori*, like the cell band formations shown in the previous section.

A case in point is the 2D test case (video provided, Video S1) where the platform is able to capture the dynamic nature of the system. Secondly, cell alignment normal to the oxygen gradient was not a part of the rule-set attributed to the cells but emerged from it. A question that suggests itself at this point is whether such behavior can be manipulated to our advantage. Thirdly, in Figures 2 and 3 (and the corresponding videos, Videos S2 and S3) – especially in Figure 3–, the concentration contours change continuously, proving the effectiveness of the platform in capturing dynamic reciprocity as defined above. A physical system with no cells inside would not show such behavior after the flow becomes stationary, beyond initial transients.

The agent-based modality of the platform relies on biological rules and therefore the relevance and accuracy with which the framework can simulate a biological system will depend upon the validity of rules attributed to the agents. The simplest ways to achieve this include recourse to the data-mining paradigm or conducting statistical analyses on the data currently existing in the literature. Such methods can assist in evaluating critical parameters of a process; for example: the minimum concentration of a chemical that cells are sensitive to, the combination of growth factors that will direct stem cells to a particular lineage, the mechanical load cells must experience to differentiate into a particular lineage etc. These methods, despite their utility, might not by themselves, however, reveal the fundamental rules in biology – that endeavor rests with experimental biologists. We feel that targeted and quantitative experimental efforts, especially guided by mathematical tools such as the ones presented here, will assist in unearthing more rules that, in association with the underlying stochastic biophysicochemical processes, govern the dynamics of biological systems.

This modeling environment, which is under continuous expansion and development, can already capture chemotaxis and cell death (necrosis as well as apoptosis). Furthermore, it can be readily used to model features such as secretion of autocrine or paracrine molecules, production of metabolic waste products, cellular polarity etc. The platform can assist in conducting a quantitative as well as a qualitative analysis of how factors such as shear stress, pressure, and availability of nutrients/soluble factors can direct differentiation of cells in any physical system – and can be therefore utilized as a design tool in the bioreactor industry during the concept selection phase. The platform can also quantify the electro-magnetic fields that may exist in a system. This can help analyze further experiments such as the ones conducted by Zhao et al (2006) [67], who investigated the impact of electric signals of physiological strength in guiding cell migration – known as galvanotaxis – and wound healing. Simulations in this direction are currently underway in our lab. The next step involves factoring in the *de* novo secretion/formation (and possibly digestion/lysis) of extra-cellular matrix by cell colonies once they aggregate beyond a certain number and attributing to the ECM a unique set of properties based on the nature of cells secreting these fibers.

The results presented in this paper are in agreement with those from other models that were discussed above. Cheng et al (2009) [16] suggested that the hydrodynamic conditions affect not only the rate, but the pattern, of tissue growth as well, something we demonstrate in this paper: the supplementary videos show that migration speed, dependent on oxygen concentration, influences growth. Furthermore, one can easily observe (Figure 5) the way transport limitations affect spatial distribution of cells [16]. According to Cheng et al (2006) [15], by inducing a preferential migration direction oxygen concentration gradients influence cell migration. The platform captured that behavior evident in any of the figures and supplementary videos. Furthermore, the impact of bioreactor/scaffold geometry on cell proliferation can be also observed.

We have developed a modeling platform that captures the cell-level as well as population-level aspects of biological systems lending the platform the capability to capture the dynamism that is the signature of biology. Through the investigation reported here we successfully tested the research hypothesis that differences in initial and boundary conditions for the same volume can lead to non-identical development of a cellular system and that our platform is capable of capturing such variation. Furthermore, the platform was validated by simulating cellular chemotaxis and comparing the results with chemotaxis of MV3 melanoma cells under FBS concentration gradient in the Insall chamber [60]. Future developments include capturing cell colonization, ECM secretion by the colonies, and attributing the ECM with relevant biophysical information (porosity, spatial heterogeneity, diffusivity to certain molecules etc.).

Conclusions

A novel way of simulating biological phenomena in bioreactors, especially dynamic reciprocity, was presented in this manuscript. The computational platform developed composed of two elements – agent-based and transport phenomena – is mature enough to model differentiation, chemotaxis and apoptosis in addition to cell proliferation, collision and persistent random walk. Most of the results discussed are in agreement with those obtained using models of similar purpose [15], [16], [21], [22]; in addition to showing behavior that may be emergent. The validated platform can be used as a design tool to test the impact of bioreactor geometries and experimental parameters on cell proliferation and differentiation in addition to supplementing the experimental techniques employed in gathering biological data.

Supporting Information

A Multi-Paradigm Modeling Framework to Simulate Dynamic Reciprocity in a Bioreactor

Showing 1/6: Video_S1.avi

Sorry we could not load your data.

Video S1.

2D test case displaying the dynamic nature of the system. The video shows proliferating cells that are being fed via medium entering the system from left hand side of the construct. Continuous cell proliferation causes a drop in the concentration of nutrient medium inducing chemotaxis in the affected population. As the supply is unable to meet the demand, cells end up undergoing hypoxia-induced apoptosis.

https://doi.org/10.1371/journal.pone.0059671.s001

(AVI)

Video S2.

Case 1 Video. The video shows results of test case 1 (discussed in the paper).

https://doi.org/10.1371/journal.pone.0059671.s002

(AVI)

Video S3.
Case 2 Video. The video shows results of test case 2 (discussed in the paper). Notice especially the continuously changing concentration contours.
https://doi.org/10.1371/journal.pone.0059671.s003
(AVI)

Video S4.
Case 3 Video. The video shows results of test case 3 (discussed in the paper).
https://doi.org/10.1371/journal.pone.0059671.s004
(AVI)

Video S5.
Case 4 Video. The video shows results of test case 4. Similar to case 3 in its geometry, the medium flow rate used for this simulation is an order of magnitude higher in comparison. The difference in boundary conditions leads to distinct cell dynamics, which results in the formation of two different cell colonies.
https://doi.org/10.1371/journal.pone.0059671.s005
(AVI)

Video S6.
Simulating chemotaxis in Insall Chamber. The video shows results of the validation experiment conducted using the virtual Insall Chamber (discussed in the paper).
https://doi.org/10.1371/journal.pone.0059671.s006
(AVI)

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Author Contributions

Developed the coupling environment for the multiparadigm modelling platform, conducted simulations and contributed to the manuscript: HK. Led the research and provided guidance regarding biological phenomena at play and specific mechanisms pertinent to existing and future bioreactors: ZC. Led the research, provided guidance regarding the computational modelling aspects of the platform, reviewed and expanded the results obtained and contributed to the manuscript preparation: YV. Conceived and designed the experiments: HK ZC YV. Performed the experiments: HK. Analyzed the data: HK YV. Contributed reagents/materials/analysis tools: HK ZC YV. Wrote the paper: HK ZC YV.

References

1. Murry CE, Keller G (2008) Differentiation of embryonic stem cells to clinically relevant populations: Lessons from embryonic development. Cell 132: 661–680.
View Article • Google Scholar

2. Freshney I, Obradovic B, Grayson W, Cannizzaro C, Vunjak-Novakovic G (2007) Principles of tissue culture and bioreactor design. In: Lanza R, Langer R, Vacanti J, editors. Principles of Tissue Engineering (3rd ed). Burlington: Elsevier Academic Press. 155–184.

3. Wendt D, Riboldi SA, Cioffi M, Martin I (2009) Bioreactors in Tissue Engineering: Scientific Challenges and Clinical Perspectives. In: Kasper C, van Griensven M, Portner R, editors. Bioreactor Systems in Tissue Engineering. Berlin: Springer-Verlag. 1–27.

4. Place ES, Evans ND, Stevens MM (2009) Complexity in biomaterials for tissue engineering. Nat Matter 8: 457–470.

View Article • Google Scholar

5. Chung CA, Yang CW, Chen CW (2006) Analysis of cell growth and diffusion in a scaffold for cartilage tissue engineering. Biotechnol Bioeng 94: 1138–1146.
View Article • Google Scholar

6. Langer R, Vacanti JP (1993) Tissue Engineering. Science 260: 920–926.
View Article • Google Scholar

7. Mertsching H, Hansmann J (2009) Bioreactor Technology in Cardiovascular Tissue Engineering In: Kasper C, van Griensven M, Portner R, editors. Bioreactor Systems in Tissue Engineering. Verlag, Berlin: Springer. 29–37.

8. Fuchs JR, Nasseri BA, Vacanti JP (2001) Tissue engineering: A 21st century solution to surgical reconstruction. Ann Thorac Surg 72: 577–591.
View Article • Google Scholar

9. Khademhosseini A, Langer R (2007) Microengineered hydrogels for tissue engineering. Biomaterials 28: 5087–5092.
View Article • Google Scholar

10. Burdick JA, Vunjak-Novakovic G (2009) Engineered microenvironments for controlled stem cell differentiation. Tissue Eng Part A 15: 205–219.
View Article • Google Scholar

11. Viswanathan S, Zandstra PW (2003) Towards predictive models of stem cell fate. Cytotechnology 41(2–3), 75–92.

12. Singh H, Hutmacher D (2009) Bioreactor studies and Computational Fluid Dynamics. In: Kasper C, van Griensven M, Portner R, editors. Bioreactor Systems in Tissue Engineering. Berlin: Springer-Verlag. 231–249.

13. Weyand B, Israelowitz M, von Schroeder H, Vogt P (2009) Fluid Dynamics in Bioreactor Design: Considerations for the Theoretical and Practical Approach. In: Kasper C, van Griensven M, Portner R, editors. Bioreactor Systems in Tissue Engineering. Berlin: Springer-Verlag. 251–268.

14. Chung CA, Lin TH, Chen SD, Huang HI (2010) Hybrid cellular automaton modeling of nutrient modulated cell growth in tissue engineering constructs. J Theor Biol 262: 267–278.
View Article • Google Scholar

15. Cheng G, Youssef BB, Markenscoff P, Zygourakis K (2006) Cell population dynamics modulate the rates of tissue growth processes. Biophys J 90: 713–724.
View Article • Google Scholar

16. Cheng G, Markenscoff P, Zygourakis K (2009) A 3D hybrid model for tissue growth: The interplay between cell population and mass transport dynamics. Biophys J 97: 401–414.
View Article • Google Scholar

17. Richmond P, Walker D, Coakley S, Romano D (2010) High performance cellular level agent-based simulation with FLAME for the GPU. Brief Bioinform 11: 334–347.
View Article • Google Scholar

18. Thorne BC, Bailey AM, Pierce SM (2007) Combining experiments with multi-cell agent-based modeling to study biological tissue patterning. Brief Bioinform 8: 245–257.
View Article • Google Scholar

19. Chavali AK, Gianchandani EP, Tung KS, Lawrence MB, Peirce SM, et al. (2008) Characterising emergent properties of immunological systems with multi-cellular rule-based computational modeling. Trends Immunol 29: 589–599.
View Article • Google Scholar

20. Lee Y, Kouvroukoglou S, McIntire LV, Zygourakis K (1995) A cellular-automaton model for the proliferation of migrating contact-inhibited cells. Biophys J 69: 1284–1298.
View Article • Google Scholar

21. Galbusera F, Cioffi A, Raimondi MT, Pietrabissa R (2007) Computational modeling of combined cell population dynamics and oxygen transport in engineered tissue subject to interstitial perfusion. Comput Methods Biomech Biomed Engin 10: 279–287.
View Article • Google Scholar

22. Galbusera F, Cioffi M, Raimondi MT (2008) An in silico bioreactor for simulating laboratory experiments in tissue engineering. Biomed Microdevices 10: 547–554.
View Article • Google Scholar

23. Farnoosh N, K Adamiak, Castle GSP (2011) 3-D Numerical Simulation of Particle Concentration Effect on a Single-wire ESP Performance for Collecting Poly-dispersed Particles. IEEE Trans Dielectr Electr Insul 18: 211–220.
View Article • Google Scholar

24. Amaziane B, El Ossmani M, Serres C (2008) Numerical modeling of the flow and transport of radionuclides in heterogeneous porous media. Comput Geosci 12: 437–449.
View Article • Google Scholar

25. Tsompanopoulou PE (2008) Performance study of GasTurbnLab, an agent-based multi-physics problem solving environment for the gas turbine engine simulation. J Comput Inf Sci Eng 8: 031008.1–031008.8.
View Article • Google Scholar

26. De Santis V, Feliziani M, Maradei F (2008) Hybrid finite element/finite difference (FE/FD) model to analyze thermal transients in biological vascularized tissues. COMPEL 27: 1307–1318.
View Article • Google Scholar

27. Portillo PM, Muzzio FJ, Ierapetritou MG (2007) Hybrid DEM-compartment modeling approach for granular mixing. AICHE J 53: 119–128.
View Article • Google Scholar

28. Lapin A, Paaschen T, Junghans K, Lubbert A (2002) Bubble column fluid dynamics, flow structures in slender columns with large-diameter ring-spargers. Chem Eng Sci 57: 1419–1424.
View Article • Google Scholar

29. Bourloutski E, Sommerfeld M (2004) Euler/Lagrange calculations of gas-liquid-solid-flows in bubble columns with phase interaction. In: Sommerfeld M, editor. Bubbly Flows: Analysis, Modelling and Calculation, Heat and Mass Transfer (series). Freyburg: Colloquium on Analysis, Modelling and Numerical Calculations of Multiphase Flow. 243–259.

30. Annaland MS, Deen NG, Kuipers JAM (2005) Numerical simulation of gas-liquid-solid flows using a combined front tracking and discrete particle method. Chem Eng Sci 60: 6188–6198.
View Article • Google Scholar

31. Galban CJ, Locke BR (1999a) Analysis of cell growth kinetics and substrate diffusion in a polymer scaffold. Biotechnol Bioeng 65: 121–132.
View Article • Google Scholar

32. Galban CJ, Locke BR (1999b) Effects of spatial variation of cells and nutrient and product concentrations coupled with product inhibition on cell growth in a polymer scaffold. Biotechnol Bioeng 64: 633–643.
View Article • Google Scholar

33. Lemon G, King JR (2006) Multiphase modeling of cell behavior on artificial scaffolds: effects of nutrient depletion and spatially non-uniform porosity. Math Med Biol 24: 57–83.
View Article • Google Scholar

34. Flaibani M, Magrofuoco E, Elvassore N (2010) Computational modeling of cell growth heterogeneity in a perfused 3D scaffold. Ind Eng Chem Res 49: 859–869.
View Article • Google Scholar

35. Lapin A, Muller D, Reuss M (2004) Dynamic behavior of microbial populations in stirred bioreactors simulated with Euler-Lagrange methods: Traveling along the lifelines of single cells. Ind Eng Chem Res 43: 4647–4656.
View Article • Google Scholar

36. Lapin A, Schmid J, Reuss M (2006) Modeling the dynamics of E-coli populations in the three-dimensional turbulent field of a stirred-tank bioreactor - A structured-segregated approach. Chem Eng Sci 61: 4783–4797.
View Article • Google Scholar

37. Lapin A, Klann M, Reuss M (2010) Multi-Scale Spatio-Temporal Modeling: Lifelines of Microorganisms in Bioreactors and Tracking Molecules in Cells. In Wittmann C, Krull R, editors. Biosystems Engineering Ii: Linking Cellular Networks and Bioprocesses. 23–43.

38. Emonet T, Macal CM, North MJ, Wickersham CE, Cluzel P (2005) AgentCell: a digital single-cell assay for bacterial chemotaxis. Bioinformatics 21: 2714–2721.
View Article • Google Scholar

39. Bonabeau E (2002) Agent-based modeling: Methods and techniques for simulating human systems. Proc Natl Acad Sci USA 99: 7280–7287.
View Article • Google Scholar

40. Bissell MJ, Hall HG, Parry G (1982) How does the extracellular-matrix direct gene-expression. J Theor Biol 99: 31–68.
View Article • Google Scholar

41. Nelson CM, Bissell MJ (2006) Of extracellular matrix, scaffolds, and signaling: Tissue architecture regulates development, homeostasis, and cancer. Annu Rev Cell Dev Biol 22: 287–309.
View Article • Google Scholar

42. Adra S, Sun T, MacNeil S, Holcombe M, Smallwood R (2010) Development of a three dimensional multiscale computational model of the human epidermis. PLoS One 5: e8511.
View Article • Google Scholar

43. Smallwood R, Holcombe M (2006) The Epitheliome Project: Multiscale agent-based modeling of epithelial cells. 3rd IEEE International Symposium on Biomedical Imaging: Macro to Nano Vols 1–3: 816–819.
View Article • Google Scholar

44. Tao S, McMinn P, Coakley S, Holcombe M, Smallwood R, et al. (2007) An integrated systems biology approach to understanding the rules of keratinocyte colony formation. J R Soc Interface 4: 1077–1092.
View Article • Google Scholar

45. Sun T, Adra S, Smallwood R, Holcombe M, MacNeil S (2009) Exploring hypotheses of the actions of TGF-beta 1 in epidermal wound healing using a 3D computational multiscale model of the human epidermis. PLoS One 4: e8515.
View Article • Google Scholar

46. Jennings NR (2000) On agent-based software engineering. Artif Intell 117: 277–296.
View Article • Google Scholar

47. Kiran M, Coakley S (2010) Flexible large-scale agent-based modeling environment user manual, University of Sheffield.

48. Ferziger J, Peric M (2002) Computational methods for fluid dynamics (3rd, illustrated ed.). New York: Springer-Verlag.

49. van Doormaal JP, Raithby GD (1984) Enhancements of the SIMPLE method for predicting incompressible fluid-flows. Numer Heat Transfer 7: 147–163.
View Article • Google Scholar

50. Lonsdale R (1993) An algebraic multigrid solver for the Navier-Stokes equations on unstructured meshes. Int J Numer Meth Heat Fluid Flow 3: 3–14.
View Article • Google Scholar

51. Patankar SV (1980) Numerical heat transfer and fluid flow. Washington; London: Hemisphere.

52. Liu T, Laurell C, Selivanova G, Lundeberg J, Nilsson P, et al. (2007) Hypoxia induces p53-dependent transactivation and Fas/CD95-dependent apoptosis. Cell Death Differ 14: 411–421.
View Article • Google Scholar

53. Lee Y (1994) Computer-assisted analysis of endothelial cell migration and proliferation. PhD, Rice Univerisity, Houston, TX.

54. Burgess BT, Myles JL, Dickinson RB (2000) Quantitative analysis of adhesion-mediated cell migration in three-dimensional gels of RGD-grafted collagen. Ann Biomed Eng 28: 110–118.
View Article • Google Scholar

55. Weidt C, Niggemann B, Hatzmann W, Zanker KS, Dittmar T (2004) Differential effects of culture conditions on the migration pattern of stromal cell-derived factor stimulated hematopoietic stem cells. Stem Cells 22: 890–896.
View Article • Google Scholar

56. Condeelis J, Singer RH, Segall JE (2005) The great escape: When cancer cells hijack the genes for chemotaxis and motility. Annu Rev Cell Dev Biol 21: 695–718.
View Article • Google Scholar

57. Stathopoulos GT, Sherrill TP, Han W, Sadikot RT, Yull FE, et al. (2008) Host nuclear factor-kappa B activation potentiates lung cancer metastasis. Mol Cancer Res 6: 364–371.
View Article • Google Scholar

58. Wang W, Wyckoff JB, Frohlich VC, Oleynikov Y, Hüttelmaier S, et al. (2002) Single cell behavior in metastatic primary mammary tumors correlated with gene expression patterns revealed by molecular profiling. Cancer Res 62: 6278–6288.
View Article • Google Scholar

59. Kedrin D, van Rheenen J, Hernandez L, Condeelis J, Segall JE (2007) Cell motility and cytoskeletal regulation in invasion and metastasis. J Mammary Gland Biol Neoplasia 12: 143–152.
View Article • Google Scholar

60. Muinonen-Martin AJ, Veltman DM, Kalna G, Insall RH (2010) An Improved Chamber for Direct Visualisation of Chemotaxis. PLoS One 5: e15309.
View Article • Google Scholar

61. Wells A (2000) Tumor invasion: Role of growth factor-induced cell motility. Adv Cancer Res 78: 31–101.
View Article • Google Scholar

62. Muinonen-Martin A “RE: Insall Chamber - PLoS One”, Message to Himanshu Kaul. Email. 20 November 2012.

63. Muinonen-Martin A “RE: Insall Chamber - PLoS One”, Message to Himanshu Kaul. Email. 21 November 2012.

64. Selivanova OM, Shiryaev VM, Tiktopulo EI, Potekhin SA, Spirin AS (2003) Compact globular structure of Thermus thermophilus ribosomal protein S1 in solution - Sedimentation and calorimetric study. J Biol Chem 278: 36311–36314.
View Article • Google Scholar

65. Guilak F, Cohen DM, Estes BT, Gimble JM, Liedtke W, et al. (2009) Control of stem cell fate by physical interactions with the extracellular matrix. Cell Stem Cell 5: 17–26.
View Article • Google Scholar

66. McBeath R, Pirone DM, Nelson CM, Bhadriraju K, Chen CS (2004) Cell shape, cytoskeletal tension, and RhoA regulate stem cell lineage commitment. Dev Cell 6: 483–495.
View Article • Google Scholar

67. Zhao M, Song B, Pu J, Wada T, Reid B, et al. (2006) Electrical signals control wound healing through phosphatidylinositol-3-OH kinase-gamma and PTEN. Nature 442: 457–460.
View Article • Google Scholar

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In Defence of a Multi-Paradigmatic Approach to Theory Development in Community Psychology

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Keywords: Theory, Science, Community Psychology, Framework, Paradigm

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In Defence of a Multi-Paradigmatic Approach to Theory Development in Community

It was once said, "There is nothing more practical than a good theory" (Lewin, 1952, p. 169) and yet Community Psychology (CP) as a practical discipline is beset with a theory-practice gulf that does not appear to be narrowing. The article by Jason, Stevens, Ram, Miller, Beasley, and Gleason (2016) plays a commendable role in outlining the challenges faced by community-based researchers and practitioners in developing, testing and utilizing theoretical approaches that could reliably benefit the health and well-being of target groups in a community. Quite rightly, Jason et al. (2016) have acknowledged that theories used in the field of CP should more accurately be termed as frameworks, rather than constituting actual theories, since theories would be expected to offer a comprehensive methodology for explaining and predicting behaviors in a range of settings. And herein lies the problem… Should the CP discipline be aimed at transposing findings, and theories, developed from research conducted in one type of social environment to a host of other potentially similar social settings? Researchers and practitioners alike may experience tensions in attempting to replicate an intervention, based on a theory, with other samples and settings. There are recent worrying trends from one study to show that with "the current (selective) publication system [in academic journals], replications may increase bias in effect size estimates" (Nuijten, et al., 2015, p.172). Likewise, we find there is a tendency in academia to avoid publishing non-significant findings (Franco, Malhotra, & Simonvits, 2014), even though a more honest and transparent approach to theory development and testing in CP would be through registration of hypotheses before a study has commenced, just as Jason et al. (2016) have endorsed. This would certainly be a way forward, but until funding agencies and academic journals are unified in their insistence for all *a priori* hypotheses to be communicated prior to conducting a study, this may be only one way to build theories that are trustworthy in the field of CP.

However, CP researchers, theorists, and practitioners face another, more pivotal challenge to being able to craft theories that can withstand tests of validity, reliability, and utility. Jason et al.'s (2016) article appears to be mainly viewed through a post-positivist "lens," which prizes numbers and the establishment of quantitative trends as the main source for theory development in CP. By reading Jason and his colleagues' (2016) citations of the heavyweights in the philosophy of science field, such as Feynman and Popper, the reader could be left wondering whether theories that have been used by CP can ever attain the same stature as theories generated by the "hard sciences." However, although some philosophers of science are quoted, an important theorist is neglected, namely Kuhn (2012), who proposed that science can progress via a process of revolutions in which paradigms influence the directions and assumptions of scientific enquiry; such paradigms are challenged and some of them can withstand such challenges. My argument here, however, is that we should not be making one paradigm – post-positivism – rule the roost in CP when there are two other paradigms that can also be influential in their own way. These two paradigms – the constructivist and the transformative (Nelson & Prilleltensky, 2010) - are vital to making progress in CP theory development and understanding how to engage in praxis by unifying the theories with community-based practices (Kagan, et al. 2011). It is through the constructivist "lens" that community practitioners and researchers can better understand another community member's world views and meaning-making and, in so doing, can work towards a theoretical understanding of how these perceptions evolve. It is through the transformative "lens" that researchers and theorists can understand how best to generate meaningful social change through activism and by engaging fully with a stakeholder group and working from an understanding of this group's interests and needs. It is through the transformative paradigm that analyses can be conducted into methodologies of effective social change and how best to implement such change, whereas the post-positivist paradigm has its utility in assessing the extent, or degree, of the changes being made. Each paradigm asks different questions, but they all play a role in seeing a social, political, and psychological phenomenon through different eyes and having a more holistic understanding of the phenomenon. By adopting a multi-paradigmatic approach, CP researchers and practitioners are less likely to be akin to the 'blind men' in the well-known parable of "The Blind Men and the Elephant" (Saxe, 1881), in which each blind man believed the elephant was solely like the body part of the elephant that was being touched at any given time and insisted his interpretation was right. On the contrary, such blind men were all correct in their own way but they were also wholly wrong by insisting that their perspective was the only correct one. Jason et al. (2016) do well in their article to recognize the role of perspectivism and that an understanding of each researcher's or theorist's perspective can be pivotal to effective and accurate theory building.

Towards the end of Jason et al.'s (2016) article, the reader is presented with an insight that argues for privilege and power to be acknowledged in relation to theory construction and research in CP. However, this seems more like an afterthought instead of being integral to how CP research and action should be conducted as a matter of course. There is also an implicit hierarchy in Jason et al.'s (2016) paper, which is evident in the discussion of cross-sectional, longitudinal, and experimental designs, but there is little mention of qualitative research methodologies, participatory action research, Fourth Generation Evaluation (Guba & Lincoln, 1989), and other mixed methods. By placing quantitative methods on a pedestal, the community-based researcher and practitioner may run the risk of doing research and action *on* a target group rather than *with*, or *on behalf of*, those in a certain target group (Williams, 2013).

By contrast, qualitative methodologies, in particular, could help CP-relevant theory generation through adopting an inductivist approach by drawing from *specific* situational and process-oriented insights that research participants have offered. From these specific data, researchers may then be able to examine the potential for transferable dynamics of social situations and interactions being experienced more generally by those in similar settings and with world views and perceptions that are also shared. Disappointingly, Jason et al. (2016) did not notice the role of grounded theory as a methodology in CP; by its very nature, grounded theory is utilized as a means whereby narratives from research participants can be transformed into a set of coding categories that are meant to show interconnectivity, and the process orientation explains how, and why, people act as they do. Although grounded theory is not a common methodology within CP-relevant research, there are good practice examples in which theory can be grounded in the perspectives of study informants (Rasmussen, et al., 2016). This inductivist approach is one way that CP can work with what matters to constituents in a sample group of interest, rather than giving undue prominence to the values and perspectives that the researcher brings to the enterprise. The inductivist approach could be a welcome antidote to the tendency in some studies to use *general* assumptions of how a social world might work and to then use the hyopothetico-deductive method to test out specific hypotheses emerging from these generalizations. This deductive approach rests on problematic assumptions, posing questions of primary interest to the researchers regardless of whether these questions interest those being researched. The resultant methodology that is deployed privileges certain dominant cultural norms and could deprive those in the target group of a voice. For instance, the 'Big Five' (Costa, Jr, Terracciano, & McCrae, 2001) is lauded by Jason et al. (2016) as having satisfactory levels of integrity, measurement rigor, and appeal. However, the Big Five is not without its criticisms (e.g. Block, 1995, 2010), not least of which is its reliance on the lexical hypothesis of personality structures being best conveyed by language used by the general public. The Big Five model also rests on the shaky foundations of not fully resolving the emic-etic tension (Dasen, 2012) of striving to find psychological universals while also needing to acknowledge the vital culture-specific influences that may often shape people's behaviors and, in turn, their psychological, emotional, and relational well-being. Models developed primarily from a Western psychological context, such as the Big Five, may often emerge from efforts to constrain its parameters to a predetermined notion of how personality should be experienced and described, rather than from conscious efforts to start from within cultures and draw upon culturally-bound language and experiences. An example of how the Big Five may not be highly valid in all cultures was an effort to translate the model into Arabic within the context of Libya; only three out of the five factors emerged after careful translation and back-translation and confirmatory factor analytic tests of this personality model (Abdelsalam, 2013).

Jason et al. (2016) make pertinent points about three CP-relevant theories that they selected out of 32 theories volunteered in a straw poll survey of users of the Society for Community Research and Action's listserv. It is not entirely clear why those three were chosen, but all three certainly have an appeal in terms of their multi-layered approach to comprehending complex social phenomena. Certainly, every researcher will have a favorite theory, and it was disappointing not to see Hobfoll's (2001) Conservation of Resources Theory mentioned, especially as it too has a multi-layered perspective by scrutinising the influences on the well-being of people by scrutinizing people as entities nested within a range of social systems. What makes Conservation of Resources theory attractive is that there are a number of hypotheses that have been stipulated *a priori* (Hobfoll, 1998) and these relate to resource loss and loss spirals, resource gain, social support, and resource appraisal. Hobfoll's theory has its roots in Ecological Theory and is it not surprising to see Bronfenbrenner's (1979) seminal approach as being at the heart of this main focus for Jason et al. (2016), especially as the Ecological Theory has such an intuitive appeal for those working in a range of communities. Jason et al. (2016) recognized the vital role for understanding how the social ecologies of microsystems, mesosystems, and macrosystems impact people's health and well-being. However, it is also noteworthy that there are other systems of which community psychologists also might need to be cognisant: the exosystem, which has indirect influences on an individual's life, and the chronosystem, which encompasses life transitions and embraces the transitory nature of a person's existence. The chronosystem is particularly pertinent to practitioners in the field of CP because social actors need to be constantly adapting to changes in their social interactions and relationships over time. Overall, the conclusion drawn by Jason et al. (2016), that the "theory" part of the Ecological Theory is perhaps less of a theory, seems to ring true. This theory (or rather, framework), with its emphasis on interdependence, cycling of resources, adaptation, and succession, is perhaps more of a metaphor for how a person's social worlds might interrelate. Yet, metaphors, by their very nature, are not literal representations of a real dynamic; they rather share similar characteristics and, owing to this, we would need to be cautious about the utility of the Ecological Theory in lending itself to the generation of testable hypotheses.

With Sense of Community theory, the challenge is balancing individual perceptions of a community of interest with that of a group's perceptions. Like Ecological Theory, sense of community as a concept seems to rely on taking more than one perspective by encompassing people as individuals and then people as aggregated groups. Empowerment Theory also encompasses this dual-pronged approach by examining how individuals can be empowered by having enriching social environments in order to flourish. Jason et al. (2016) have noted the inherent tensions if an individual's empowerment capabilities are not fostered by an organization and where there could be the contradiction of having an organization that evinces empowerment among many of its members, but not all of them. This dynamic brings to mind processes of group-think (Janis, 1982) and team-think (Manz & Neck, 1997) in which considerable pressure is brought to bear on team members to conform to group norms and ritualised behaviors.

Overall, Jason et al. (2016) have depicted a compelling argument that the CP discipline is bereft of theories that can withstand clear tests of: being amenable to *a priori* hypothesis generation, possessing unambiguous operationalization of concepts, and being replicable in a wide range of settings and situations. Instead, it is evident from Jason and his team's (2016) arguments that they believe there is much to be achieved before commonly used frameworks and models in the field of CP can attain the status of being theory-like. Where Jason et al. (2016) and I diverge is the method for achieving better quality theories in CP. Although quantitative data collection and analysis, born mainly out of the post-positivist enterprise, can offer a great deal of understanding of the breadth of people's experiences, they cannot offer the depth of insight and the considerable potential for social change that the respective constructivist and transformative paradigms can offer. A better route for theory relevant to community-based researchers and practitioners is through adopting a practice that should become increasingly more common: utilizing mixed methods to research and to embrace multiple paradigms simultaneously. In doing so, tangible and testable theories can be sculpted to form the basis of making a real difference to people's lives.

References

Abdelsalam, A.A. (2013). *The Personal Characteristics of University Lecturers in Libyan Universities*. Unpublished PhD thesis, Nottingham Trent University, United Kingdom.

Block, J. (1995). A contrarian view of the five-factor approach to personality description. *Psychological Bulletin, 117*, 187-215.

Block, J. (2010). The Five-Factor framing of personality and beyond: Some ruminations. *Psychological Inquiry, 21*, 2–25.

Bronfenbrenner, U. (1979). *The ecology of human development: Experiments by nature and design*. Cambridge, MA: Harvard University Press.

Costa, Jr., P.T., Terracciano, A., & McCrae, R.R. (2001). Gender differences in personality traits across cultures: Robust and surprising findings. *Journal of Personality and Social Psychology, 81*, 322–331.

Dasen, P. R. (2012). Emics and etics in cross-cultural psychology: towards a convergence in the study of cognitive styles. In T.M.S. Tchombe, A. B. Nsamenang, H. Keller and M. Fülöp (Eds.) *Cross-cultural psychology: An Africentric perspective.* (pp. 55-73). (Proceedings of the 4th Africa Region Conference of the IACCP, University of Buea, Cameroun, Aug. 1-8, 2009.) Limbe, Cameroun: Design House.

Franco, A., Malhotra, N. & Simonovits, G. (2014). Publication bias in the social sciences: Unlocking the file drawer. *Science, 345*, 1502-1505.

Guba, E. G., & Lincoln, Y. S. (1989). *Fourth generation evaluation*. London: Sage.

Hobfoll, S.E. (1998). *Stress, culture, and community: The psychology and philosophy of stress*. New York: Plenum.

Hobfoll, S. E. (2001). The influence of culture, community, and the nested-self in the stress process: Advancing conservation of resources theory. *Applied Psychology, 50*, 337-421.

Janis, I. L. (1982). *Groupthink: Psychological Studies of Policy Decisions and Fiascoes*. Boston: Houghton Mifflin.

Jason, L. A., Stevens, E., Ram, D., Miller, S. A., Beasley, C. R., & Gleason, K. (2016). Theories in the field of community psychology. *Global Journal of Community Psychology Practice. 7*(2), pp. 1-27.

Kagan, C., Burton, M., Duckett, P., Lawthom, R., Siddiquee, A. (2011). *Critical community psychology*. Chichester: Wiley.

Kuhn, T.S. (2012). *The Structure of Scientific Revolutions: 50th Anniversary Edition*. Chicago: University of Chicago Press.

Lewin, K. (1952*). Field theory in social science: Selected theoretical papers by Kurt Lewin*. London: Tavistock.

Manz, C.C. & Neck, C.P. (1997). Teamthink: beyond the groupthink syndrome in self-managing work teams, *Team Performance Management: An International Journal, 3*(1), 18-31.

Nelson, G. & Prilleltensky, I. (2010). *Community Psychology: In Pursuit of Liberation and Well-being*. 2nd edition. New York: Palgrave Macmillan.

Nuijten, M. B., van Assen, M. A., Veldkamp, C. L., & Wicherts, J. M. (2015). The Replication Paradox: Combining Studies can Decrease Accuracy of Effect Size Estimates. *Review of General Psychology, 19*(2), 172-182.

Rasmussen, A., Akinsulure-Smith, A.M., & Chu, T. (2016). Grounded theory. In L. A. Jason and D. S. Glenwick (Eds.). *Handbook of methodological approaches to community-based research: Qualitative, quantitative, and mixed methods*. New York, N.Y.: Oxford University Press.

Saxe, J.G. (1881). *The Poems of John Godfrey Saxe* (Highgate Edition). Boston: Houghton, Mifflin and Company.

Williams, G.A. (2013). Doing Community Psychology Research with People and For People, Rather than On People - Challenges and Ways Forward. Keynote presentation at *BPS Community Psychology Section AGM, December 16, 2013*, London, United Kingdom.

multiparadigmatic

English

Etymology

multi- + *paradigmatic*

Adjective

multiparadigmatic (*not comparable*)

1. Using or conforming to more than one paradigm.

paradigm

Contents

English

WOTD – 13 June 2006

Alternative forms

- paradigma (*archaic*)

Etymology

Established 1475-85 from Late Latin *paradīgma*, from Ancient Greek παράδειγμα (*parádeigma*, “pattern”), from παραδείκνυμι (*paradeíknumi*, “I show [beside] or compare”) + -μα (*-ma*, “*forming nouns concerning the results of actions*”).

Pronunciation

- (*UK*) IPA(key): /ˈpæɹ.ə.daɪm/
- (*US*) enPR: ˈpărədīm, IPA(key): /ˈpæɹ.ə.daɪm/, /ˈpɛɹ.ə.daɪm/, /ˈpeɪ.ɹə.daɪm/

  (Mary–marry–merry *merger*) Audio (US) (file)

- (*General Australian*) IPA(key): /ˈpæɹ.ə.dɑɪm/
  - Audio (AU) (file)

Noun

paradigm (*plural* **paradigms** *or* **paradigmata**)

1. A pattern, a way of doing something, *especially* (*now often derogatory*) a pattern of thought, a system of beliefs, a conceptual framework.

   Synonyms: style, model, worldview
   *Thomas Kuhn's landmark "The Structure of Scientific Revolutions" got people talking about **paradigm** shifts, to the point the word itself now suggests an incomplete or biased perspective.*

2. An example serving as the model for such a pattern.

   Synonyms: template, exemplar, posterboy

   - **2000**, *Estate of William F. Jenkins v. Paramount Pictures Corp.*:

     According to the Fourth Circuit, "Coca-Cola" is "the **paradigm** of a descriptive mark that has acquired secondary meaning".

   - **2003**, Nicholas Asher, Alex Lascarides, *Logics of Conversation*, Cambridge University Press, →ISBN, page 46:

     DRT is a **paradigm** example of a dynamic semantic theory, […]

3. (*linguistics*) A set of all forms which contain a common element, especially the set of all inflectional forms of a word or a particular grammatical category.

   *The **paradigm** of "to sing" is "sing, sang, sung". The verb "to ring" follows the same **paradigm**.*

Synonyms

- (*exemplar*): Thesaurus:exemplar, Thesaurus:model

Derived terms

- morphoparadigm
- multi-paradigm
- paradigmatic
- paradigmaticism
- paradigm leveling
- paradigm shift
- social conflict paradigm

Translations

way of viewing reality

- Armenian: հարացույց (hy) (haracʿuycʿ)
- Catalan: paradigma (ca) *m*
- Chinese:

  Mandarin: 範式／范式 (zh) (fànshì)

- Czech: paradigma (cs) *n*, pojetí (cs) *n*
- Danish: paradigme (da) *n*
- Dutch: paradigma (nl) *n*, denkkader (nl) *n*
- Finnish: paradigma (fi), maailmankatsomus (fi)

- French: paradigme (fr) *m*
- German: Paradigma (de) *n*, Weltanschauung (de) *f*, Bezugssystem (de) *n*, Sicht der Dinge *f*, Denkrahmen *m*
- Iban: paradigma
- Icelandic: hugarfar (is) *n*
- Indonesian: paradigma (id)
- Italian: paradigma (it) *m*
- Kazakh: парадигма (paradigma)
- Kyrgyz: парадигма (paradigma)
- Macedonian: пара́дигма *f* (paradígma)
- Malay: paradigma
- Norwegian:

  Bokmål: paradigme (no) *n*, paradigma *n*
  Nynorsk: paradigme *n*, paradigma *n*

- Polish: paradygmat (pl) *m*
- Portuguese: paradigma (pt) *m*
- Russian: пара́дигма (ru) *f* (paradígma)
- Slovak: paradigma *f*
- Spanish: paradigma (es) *m*
- Swedish: paradigm (sv) *n*
- Turkish: paradigma (tr)

example serving as a model or pattern

- Arabic: نُموذج, مِثَال (miṯāl), آيَة (ar) (ʔāya)
- Armenian: հարացույց (hy) (haracʻuycʻ)
- Bulgarian: образец (bg) *m* (obrazec), пример (bg) *m* (primer)
- Catalan: paradigma (ca) *m*
- Chinese:

  Mandarin: 範例／范例 (zh) (fànlì), 模範／模范 (zh) (mófàn), 典範／典范 (zh) (diǎnfàn)

- Czech: paradigma (cs) *n*
- Dutch: paradigma (nl) *n*
- Finnish: paradigma (fi), ajatusmalli
- French: paradigme (fr) *m*
- German: Beispiel (de) *n*, Musterbeispiel (de) *n*
- Hebrew: פָּרָדִיגְמָה (he) *f* (paradigma)
- Iban: paradigma
- Icelandic: fyrirmynd (is) *f*, viðmið *n*
- Indonesian: paradigma (id)
- Italian: paradigma (it) *m*
- Japanese: 模範 (ja) (もはん, mohan)
- Macedonian: пара́дигма *f* (paradígma)
- Malay: paradigma
- Polish: paradygmat (pl) *m*

- Portuguese: paradigma (pt) m
- Romanian: paradigmă (ro) f
- Russian: паради́гма (ru) f (paradígma), образе́ц (ru) m (obrazéc), приме́р (ru) m (primér)
- Spanish: paradigma (es) m
- Turkish: paradigma (tr)

linguistics: all forms which contain a common element

- Arabic: قياس (عِلم الصرْف)
- Armenian: հարացույց (hy) (haracʿuycʿ)
- Bulgarian: парадигма (bg) f (paradigma)
- Catalan: paradigma (ca) m
- Chinese:

  Mandarin: 詞形變化表／词形变化表 (cíxíng biànhuàbiǎo)

- Czech: vzor (cs) m
- Danish: paradigme (da) n
- Dutch: paradigma (nl) n
- Faroese: bendingarmynstur n
- Finnish: paradigma (fi), taivutuskaava (fi), muotosarja (fi)
- French: paradigme (fr) m
- Georgian: პარადიგმა (ka) (ṗaradigma)
- German: Paradigma (de) n, Flexionsmuster (de) n, Flexionsschema n
- Greek: παράδειγμα (el) n (parádeigma)

  Ancient: παράδειγμα n (parádeigma)

- Iban: paradigma
- Icelandic: beygingardæmi (is) n
- Indonesian: paradigma (id)
- Italian: paradigma (it)
- Japanese: 語形変化表 (ごけいへんかひょう, gokei henkahyō)
- Malay: paradigma
- Norwegian:

  Bokmål: paradigme (no) n, paradigma n
  Nynorsk: paradigme n, paradigma n

- Polish: paradygmat (pl) m
- Portuguese: paradigma (pt) m
- Russian: паради́гма (ru) f (paradígma)
- Slovak: vzor m
- Spanish: paradigma (es) m
- Turkish: paradigma (tr)

The translations below need to be checked and inserted above into the appropriate translation tables. See instructions at Wiktionary:Entry layout § Translations.

Translations to be checked

- Korean: (please verify) 패러다임 (paereodaim)

References

- “paradigm”, in *The American Heritage Dictionary of the English Language*, 4th edition, Boston, Mass.: Houghton Mifflin, 2000, →ISBN.
- “paradigm (https://www.dictionary.com/browse/paradigm)”, in *Dictionary.com Unabridged*, Dictionary.com, LLC, 1995–present.
- "paradigm (http://wordnetweb.princeton.edu/perl/webwn?s=paradigm)" in *WordNet 2.0*, Princeton University, 2003.

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Framing the Human Dimensions of Mountain Systems: Integrating Social Science Paradigms for a Global Network of Mountain Observatories

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The Global Network of Mountain Observatories (GNOMO) is an international initiative seeking to increase communication and collaboration and align methodologies to assess commonalities and differences across the world's mountain landscapes. Oriented toward sustainable mountain development, GNOMO requires the integration of social and natural sciences, as well as a diverse array of stakeholder perspectives. This paper highlights challenges associated with integrating social sciences because of the inherent paradigmatic differences within the social sciences. The value orientations of mountain researchers, as well as the divergent societal and institutional values regarding mountains, create a need for new approaches to observing mountain landscapes. A framework is presented to organize complex information about mountain social–ecological systems based on human conditions (from vulnerability to wellbeing), environmental actions (from degradation to stewardship), and environmental conditions that vary across time, space, and scales. A multiparadigmatic, multimethod approach is proposed to combine theory-driven quantitative indicators, qualitative perspectives from diverse knowledge standpoints, and critical inquiries into power relationships to fully represent dynamic mountain systems.

Keywords: *Social science; mountain observatories; paradigms; sustainable mountain development; vulnerability; wellbeing; environmental action.*

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Introduction

Mountain landscapes are widely acknowledged to have local, regional, national, and global significance for reasons ranging from cultural identity to natural resource and biodiversity provision (Debarbieux and Price 2008). For at least a quarter of a century, international effort has focused on coordinating scientific endeavors with regard to sustainable mountain development around the world (UNCED 1992; Debarbieux and Price 2008; Messerli 2012; UN 2015). More recently, the Mountain Research Initiative and others have led an effort to build a network of observatories focused on the sustainability of mountain social and ecological systems around the world (Greenwood 2013). The Global Network of Mountain Observatories (GNOMO) (http://gnomo.ucnrs.org) has emerged as an interdisciplinary effort to increase communication and collaboration and align methodologies to assess commonalities and differences across the world's mountain landscapes. The pursuit of global research platforms to support sustainability led by the Future Earth initiative calls for full integration of scientific disciplines, coproduction of knowledge with societal partners, and development of new insights, data, and tools to help address global challenges (Future Earth 2014). Yet the challenges of such interdisciplinary and transdisciplinary approaches, particularly the inclusion of social sciences, are often profound (Kinzig 2001; Strang 2009; Mooney et al 2013; Brown et al 2015).

The mountain research community has long recognized the importance of mountains to people and communities, the environmental and social impacts of human actions, and the broader cognitive, cultural, political, economic, and ecological dimensions of mountains (Price 1986; Messerli and Ives 1997; Price et al 2013). The GNOMO initiative shares the Future Earth perspective that sustainable mountain development requires a holistic understanding and comparison of social–ecological systems. Yet the systematic inclusion of the social sciences in mountain observatory efforts has lagged behind that of the biophysical sciences (Björnsen Gurung et al 2012; Greenwood 2013). This paper explores the challenge of integrating the social sciences into the mountain research agenda, and into the GNOMO effort specifically, by highlighting complexity within the social sciences and the need to recognize the fundamental role of values in science and society in driving human–nature relationships in mountain landscapes. An agenda is offered here and organized according to a multiparadigmatic and multimethod framework to help the mountain research community meet interdisciplinary and transdisciplinary goals associated with sustainable mountain development.

What are the challenges of integrating social science approaches?

The call for integrating natural and social sciences to understand social–ecological systems is not new (Kinzig 2001), and mountain landscapes have been presented as a logical focal point for such integration (Freudenburg et al 1995; Price et al 2013). Yet the integration of natural and social sciences continues to be a challenge. MacMynowski (2009) suggested, "The two discussions are running in parallel with stunningly little crossover." Kinzig (2001: 715) wrote, "We will have to overcome or dismantle several barriers to such research" and "Our biggest challenge will lie in seeing what we discover in the process." Brown et al (2015) pointed to conflictual power dynamics and misinterpretations between social and natural scientists. The conjoint constitution of and contingent interconnections among physical and social mountain landscape characteristics varying across time and space make it imperative that these sciences be integrated for sound assessment and understanding (Freudenburg et al 1995).

In the mountain research community, there are signs of progress. Natural and social scientists have come together at conferences in recent years to pursue understanding of mountain systems and to establish GNOMO (eg Perth III: Mountains of Our Future Earth in Perth, Scotland, in 2015, and the Global Fair and Workshop on Mountain Observatories in Reno, Nevada, USA, in 2014). However, despite having these venues for scientific integration, full collaboration and coupling of human–natural systems through interdisciplinary science remains elusive.

The pursuit of GNOMO raises the question of what to observe and how; the answer is often framed from the vantage point of the observers (Williams 2014). In other words, what mountain researchers deem important to observe is likely to differ depending on their experiences and perspectives. Within the earth and natural sciences, shared adherence to scientific methods and underlying laws regarding how mountain biophysical systems function creates more common ground for interdisciplinary research. Within the social sciences, however, there are even stronger underlying ideological boundaries and more competing ways of making sense of the world than there are in the natural sciences (Westley et al 2001).

Different disciplinary languages, focal points, traditions, and methods exist, along with deep divisions among scientific paradigms, leading to seemingly irreconcilable differences about how the social world works and how it can and should be observed—and, in turn, about what aspects of mountain social systems should be observed and how this should be done. This can confuse and frustrate the integrative process, particularly when awareness of these differences is low. Thus, a key challenge for the integration of social science into mountain observatory efforts is that of integrating the social sciences themselves.

Approaches to social science can be loosely grouped under 3 paradigms, with the caveat that there are myriad hybrid and alternative approaches in practice:

1. *Positivist* (also known as realist) approaches are premised on the notion that there are observable, measurable realities in the social world (Neuman 2006). Much like biophysical science approaches, positivist observations are guided by theory and hypothesis testing with the goal of generalization and classification, and quantitative methods are common. This deductive approach to science works well when relative concepts and hypotheses are well understood and operationalized (Bliss 1999).
2. *Constructivist* approaches emphasize subjective meanings constructed in context; methodologically, they focus on capturing relevant voices and assessing values and lived experiences (Irwin 2001; Neuman 2006). This more inductive approach—taken to explore patterns and processes through observation to build, rather than test, theory—often incorporates more qualitative research methods and analysis (Bliss 1999).
3. *Critical* social science approaches focus on theories of macro-level power dynamics and social structures that enable or constrain capacities of actors in social systems to illuminate injustices and change society (Neuman 2006). While often more abstract and highly theoretical in general, critical social science approaches applied to environmental and natural resource issues, as in political ecology, incorporate empirical qualitative or quantitative data to assess power relationships and institutions (Scoones 1999; Robbins 2011). Critical theorists may be strongly theory driven, like positivists, but they accept the premise of social constructions of reality and do not assume their work is objective.

These 3 broad approaches to social science represent different ways of finding meaning in social phenomena. Researchers tend to be firmly entrenched within one of them, and lines of distinction are often intellectual battlegrounds despite urgings to "unthink our intellectual fetters" (Wallerstein 1991: ix). These tensions find their way into processes such as the pursuit of a global network of mountain observatories. Untangling them is key to finding a balance between local relevance and generalization (Peralvo and Bustamante 2014).

Science for sustainable mountain development is value driven

The mountain observatory effort is tied to the mission of sustainable development (Greenwood 2013). What should be sustained and developed are questions of value (Leiserowitz et al 2006). Values and attitudes are uncomfortable spaces for positivists and natural scientists who claim to work in the realm of facts and objectivity, yet accepting the importance of reflexivity is key to transforming science for sustainable development (Kläy et al 2015).

Recent survey data obtained by the author and the Mountain Research Initiative from participants attending the Perth III: Mountains of Our Future Earth conference in Scotland in October 2015 (Gleeson et al 2016, in this issue) suggest that biophysical and social scientists alike hold strong values about mountains. This shared affinity for mountain landscapes may create common ground among mountain researchers, despite paradigmatic and disciplinary differences. An overwhelming majority (80%) of 302 survey respondents (82% of biophysical scientists and 78% of social scientists) indicated agreement with the statement "Mountains have special meaning or personal value to me." We tend to study what we are interested in and care about, but this raises the questions of whether we might be reifying mountains as operating under unique processes and whether we might have an underlying normative perspective in our science, driven by what we believe should be studied and why, rather than merely how things work. Thinking about our "positionality" or situated vantage point as mountain researchers is important:

> *All observers may attain only a partial or incomplete comprehension of the world due to their embedded and inevitable positionality within any particular province of spatial–temporal reality. This applies both to so-called objective scientific observers who seek to stand apart from the world and to people going through their daily lives embedded in concrete places.*
>
> (Williams 2014: 75)

Given that mountain researchers come to the observation of mountain social–ecological systems with emotion, values, and norms about what the goals of sustainable mountain development should be, opening the logic of scientific inquiry and observation beyond hypotheticodeductive methods to more inductive ways of thinking is essential (Wu 2006).

Observing mountain landscapes inherently extends the importance of mountain values to other people—in addition to scientific researchers—who live and work in mountains, because they also hold values, experiences, and identities attached to mountains as places and home. Those who visit mountains for recreation or other amenities are also motivated by values, and these may or may not be compatible with those of local people. People, institutions, and industries have different resource-related and financial interests based on different perspectives on the relationship between humans and nature (Flint et al 2013). Flows of ecosystem services spread far beyond what we might delineate as mountain landscapes, given regional and global interactions and connections (Grêt-Regamey et al 2012). There are both synergies and tradeoffs among these values. While some of these landscape, resource, or ecosystem values can be monetized or at least quantified, some cannot, and in some instances, to try to do so is deemed hostile or offensive (Gómez-Baggethun and de Groot 2010). Assessing the economic, social, and ecological costs and benefits associated with actions taken to advance diverse environmental values requires integrating knowledge from across disciplinary divides and beyond science to fully embrace a transdisciplinary approach to sustainable mountain development.

Proposing an integrated environmental social science framework

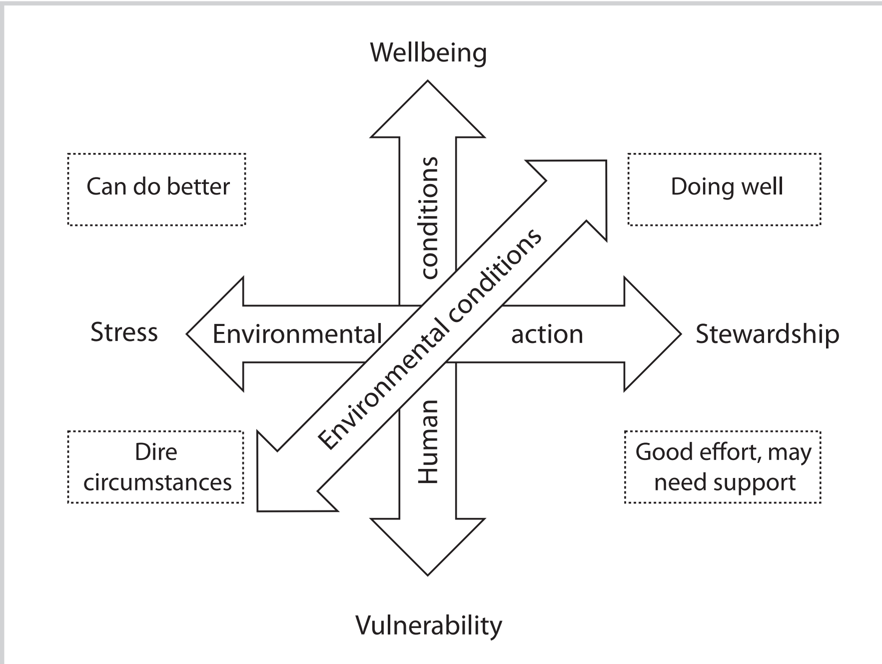
While the paradigmatic differences within the social sciences are challenging, there are examples of interparadigmatic integration for understanding patterns, processes, and change in social–ecological systems. The more successful efforts focus on nomothetic or general orienting concepts such as resilience, rather than on specific disciplines, theories, methods, contexts, and units of analysis. As GNOMO seeks to improve understanding of what is generalizable and what is context-specific across mountain landscapes, we need overarching concepts and innovative ways to combine paradigms and methodologies. Within general conceptual space, however, space should remain for individuals or teams to engage in their own research endeavors. A framework structured around key concepts can transcend disciplinary differences and provide an adaptive structure to the mountain observatory initiative.

One such framework is offered here (Figure 1). It combines two human dimensions—conditions of wellbeing and vulnerability and environmental choices leading to degradation or stewardship—and a third dimension of biophysical conditions in the environment. All 3 dimensions are dynamic across time, space, and scale and frame components of mountain observations that together can be used to assess or guide progress toward sustainable development. It would enable mountain observatories to take into account historical experience and future projections or goals, heterogeneity across places, and scales from individual and local to national and transnational.

Human conditions (wellbeing and vulnerability)

Social science mountain researchers often seek to make sense of changes in the wellbeing of individuals, communities, and governance systems in and across mountain landscapes. Depending on their disciplinary orientation, this may involve assessing health, livelihoods, happiness, relationships (social wellbeing), prosperity

FIGURE 1 Basic framework for observing the human dimensions of mountain development.



(economic wellbeing), governance capacity, or justice. Several well-known indices have quantified such indicators—including the International Organisation for Economic Co-operation and Development's Better Life Index (OECD 2016), which offers 11 dimensions and 24 indicators; the US Environmental Protection Agency's Human Wellbeing Index, with 8 domains (similar to OECD dimensions), 25 indicators, and 79 metrics (Summers et al 2014); and the United Nations Development Programme's Human Development Index (UNDP 2016), which contains just 3 indicators (Table 1). These indices represent positivist approaches to wellbeing—with vast differences in variables, how the variables are weighted in different global contexts, and the availability of the information they seek to measure.

Taking a more constructivist orientation, Larson et al (2015) suggested that community wellbeing should be the focal point of inquiry, providing a context for combining individual, social, and ecological dimensions of wellbeing. Common ground perceived among people sharing a common purpose, identity, and place forms a foundation for community wellbeing that is uniquely contextual in experience (Wilkinson 1991). The notion of wellbeing provides a unifying dimension for observation that allows people from different disciplines and paradigms to communicate and work together. Placed in this relatively simple framework, details, nuances, and differences become greater than the sum of their parts and provide a more holistic picture than would be possible within a single discipline or paradigm (Pohl and Hirsch Hadorn 2007).

Regarding vulnerability, there is consensus that exposure and sensitivity to harmful stressors combine to create vulnerabilities that are offset by adaptive capacities and that this vulnerability nexus is influenced by change drivers at multiple scales (Prosperi et al 2014). Social and biophysical vulnerability, like wellbeing (as illustrated earlier), are often operationalized and measured with quantitative indicators (Cutter et al 2003; De Lange et al 2010). However, Eakin and Luers (2006: 388) cautioned against a formulaic interpretation of vulnerability: "Vulnerability assessments thus appear most successful—or perhaps most relevant—when they are conducted for defined human–environment systems, particular places, and with particular stakeholders in mind."

Given that what is perceived to be real is real in its consequences (Thomas and Thomas 1928), the subjective interpretations or social constructions of vulnerability, such as risk perceptions, experiences, and forward-looking scenario assessments, are important to observe in mountain landscapes, as well as the quantitative, measurable indicators of processes and conditions. Furthermore, critical social science approaches investigate how power dynamics influence inequities in vulnerability, as well as adaptive capacities to mitigate risks, and where changes might lead to more sustainable options. Within the conceptual space of vulnerability and wellbeing, social scientists from different disciplinary and paradigmatic orientations can contribute to mountain observatories to fully document past and current conditions, as well as future trajectories.

TABLE 1 Key wellbeing indices and their indicators.

Better Life Index (OECD)[a]	Human Wellbeing Index (US Environmental Protection Agency)[b]	Human Development Index (UNDP)[c]
Health Life expectancy, self-reported health	**Health** Population with a regular family doctor, satisfaction with healthcare, asthma mortality, cancer mortality, diabetes mortality, heart disease mortality, infant mortality, life expectancy, suicide mortality, alcohol consumption, healthy behaviors index, teen pregnancy, teen smoking rate, happiness, life satisfaction, perceived health, adult asthma prevalence, cancer prevalence, childhood asthma prevalence, coronary heart disease prevalence, depression prevalence, diabetes prevalence, heart attack prevalence, obesity prevalence, stroke prevalence	**Life expectancy at birth**
Education Educational attainment, student skills, years in education	**Education** Mathematics skills, reading skills, science skills, adult literacy, high school completion, participation, postsecondary attainment, bullying, contextual factors, physical health, social relationships and emotional wellbeing	**Education** Mean years of schooling for adults aged 25 years, expected years of schooling for children of school-entering age
Income Household net adjusted disposable income, household net financial wealth **Jobs** Employment rate, job security, long-term unemployment rate, personal earnings	**Living standards** Food security, housing affordability, incidence of low income, median household income, persistence of low income, median home value, mortgage debt, job quality, job satisfaction	**Standard of living** Gross national income per capita
Housing Dwellings without basic facilities, housing expenditure, rooms per person	—	—
Community Quality of support network	**Social cohesion** Belonging to community, city satisfaction, discrimination, helping others, trust, interest in politics, registered voters, satisfaction with democracy, trust in government, voice in government decisions, voter turnout, extended screen time guidelines, frequency of meals at home, parent–child reading activities, participation in group activities, participation in organized extracurricular activities, volunteering, close friends and family, emotional support	—
Civic engagement/governance Consultation on rule-making, voter turnout	—	—
Environment Air pollution, water quality	**Connection to nature** Connection to life, spiritual fulfillment	—
Safety Assault rate, homicide rate	**Safety and security** Accidental morbidity and mortality, loss of human life, property crime, violent crime, community safety, social vulnerability index	—
Life satisfaction	**Spiritual and cultural fulfillment** Performing arts attendance, rate of congregational adherence	—
Work–life balance Employees working long hours, time devoted to leisure and personal care	**Leisure time** Average nights on vacation, physical activity, leisure activities, adults who provide care to seniors, adults working long hours, adults working standard hours	—

[a] OECD 2016.
[b] Summers et al 2014.
[c] UNDP 2016.

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Environmental actions (degradation and stewardship)

Examining actions and resulting conditions over time under various circumstances of human action provides longitudinal assessments of trends, anomalies or surprises, and emergent issues. There are commonly accepted ways of measuring and classifying the impact of environmental actions as degradation or stewardship. Indicator-based approaches such as the Ecological Footprint (Holmberg et al 1999) or the US Environmental Protection Agency's Environmental Quality Index, designed to account for environmental hazards in built and natural environments and associations with adverse health effects at the county scale (Messer et al 2014), are 2 examples among many at multiple scales around the world for assessing the environmental consequences of human actions. What is needed for GNOMO, however, is a classification scheme or typology to describe not only the impacts of human activity on the environment but also the array of environmental actions undertaken, along with their motivations, that lead to outcomes or changes along an environmental degradation–stewardship continuum. Globally relevant indicators or assessments of environmental action will likely need place-based interpretation for contextualization. For example, community-based natural resource management is a type of collective environmental action that may have varying environmental outcomes or impacts around the world (Kumar 2005).

Integrated approach

Coupling the social science assessment of environmental actions with biophysical assessment of environmental conditions is essential for full coupling of the social–ecological system; it requires the integration of the social sciences and of the social and natural sciences (Lassoie and Sherman 2010). An integrated approach that connects observations made from multiple social science paradigms with environmental conditions may help to differentiate mountain places, communities, and landscapes that are in dire circumstances, are making good effort but needing support, have the capacity to do better, or are doing well on the road to sustainability (Figure 1). In this way, the framework for integrating environmental social sciences into mountain observation may not only improve the robustness of scientific assessments but also inform policy- and decision-makers.

How to integrate social science in mountain research for sustainable development

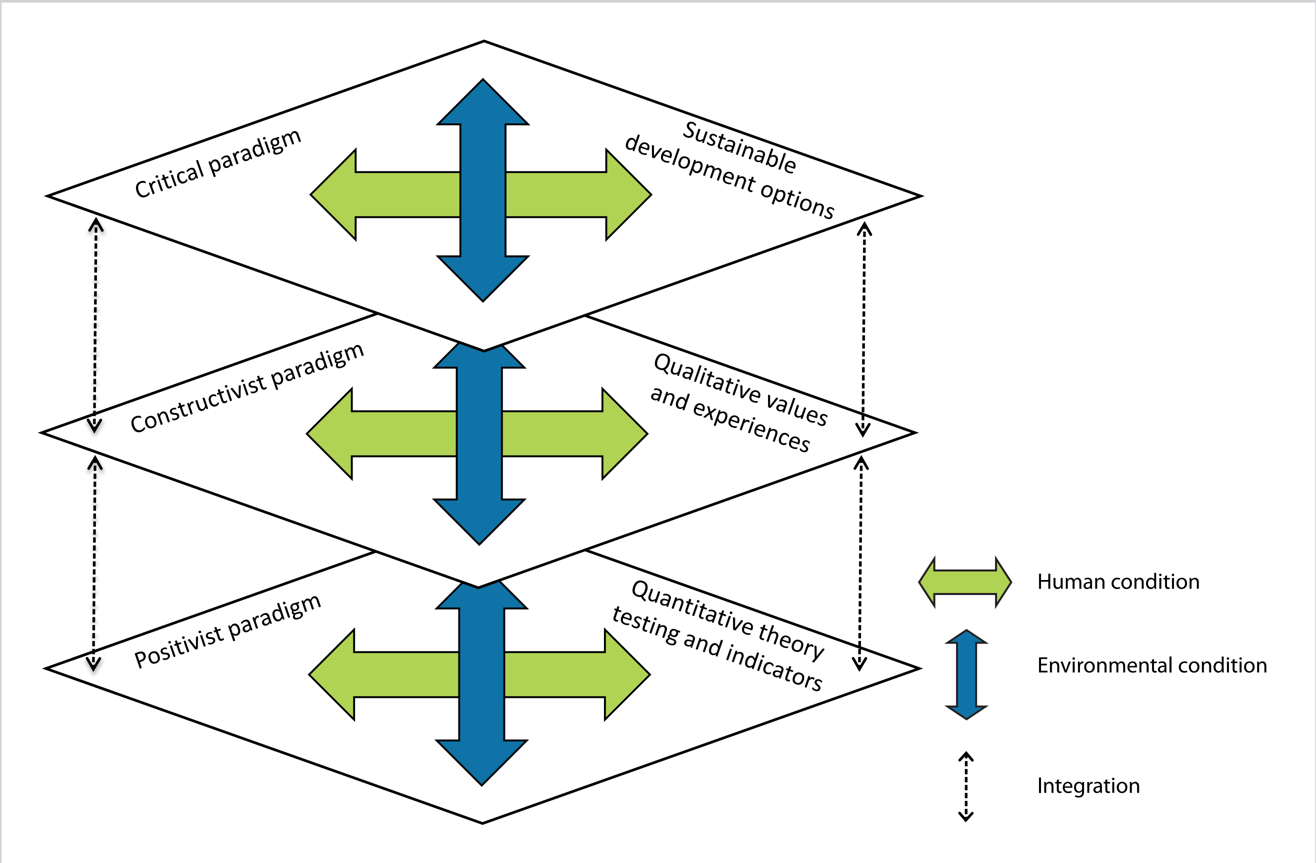
Breaking down disciplinary and paradigmatic barriers to integrate social science approaches for more holistic and comparative understanding is essential for a robust global network of mountain observatories. A mixed-methodological approach emphasizes a combination of "diverse ways of thinking, knowing, and valuing" (Greene and Caracelli 2003: 93) and rejects the notion that one paradigm is better than another, which has been a fundamental barrier to interdisciplinarity (Brown et al 2015). The inclusion of constructivist and critical approaches, along with their associated methodologies, in mountain observation will lead to more engagement with values and power dynamics than typically found in traditional positivist science. This is essential for addressing questions of what to sustain and develop in mountain social–ecological systems and how to diversify the voices and perspectives included in observations. An integrated, eclectic toolbox of methods will help assess multiple conditions, actions, and their implications, along with locally relevant values, meanings, and experiences to help facilitate dialogue, collaboration, and complex decision-making.

The previously outlined framework can be operationalized using methods that draw on the 3 paradigms outlined earlier—positivist, constructivist, and critical—to represent the human dimensions of mountain systems. These can be thought of as different layers of the same research effort (Figure 2). Just as an interdisciplinary effort brings multiple researchers together, this framework requires a community of researchers who accept that science can be done by integrating different epistemologies and ontologies to collectively observe social systems in mountains.

The positivist layer organizes bundles of indicators and theory-driven formulae to measure wellbeing, vulnerability, environmental degradation, and environmental stewardship at different scales across space and over time. Premised on the assumption that there are observable realities in the social world that can be measured quantitatively, this provides a data-driven picture of what is happening where. An example of a conceptual framework and associated structural variables for assessing governance in varying action situations is the social–ecological systems framework (Ostrom 2009) and its elaboration into the institutional analysis and development framework (Ostrom 2011). However, the quantification and classification of structural information is less helpful in explaining why patterns and processes are occurring when and where they are found and risks overgeneralization and blind spots, leading to omission of important locally relevant variables in environmental observatory models (Freudenburg 1996).

The constructivist layer incorporates values, meanings, experiences, and motivations across diverse perspectives within mountain social systems. This research assumes social meanings and motivations are constructed in context. By emphasizing the voices, lived experiences, and motivations of individuals, social groups, and institutions within mountain landscapes, engaged and participatory research builds a mosaic of contextual perspectives, shedding light on contested or shared interpretations of

FIGURE 2 Multiparadigmatic framework for observing the human dimensions of mountain development.



vulnerability, wellbeing, and environmental actions from degradation to stewardship. The Mountain Voices oral history project (Panos Oral Testimony Programme n.d.) is an international application of a constructivist approach to mountain development and associated vulnerabilities. While useful for capturing the deep meanings held in places (Geertz 2000), representation across societies and spaces can be difficult. The risk of overreliance on this type of information alone is relativism or limited application beyond a given location, though this can be overcome to an extent through meta-analytical, comparative research. Integrating positivist and constructivist approaches will help to triangulate findings from different vantage points for deeper understanding.

The critical layer reveals unequal distributions of environmental costs and benefits, with a view to changing social order or improving socioenvironmental conditions (Robbins 2011). Social science that empirically reveals power relationships and factors enabling or constraining actions can help to identify steps that could be taken to implement change in systems that may improve conditions within mountain communities, landscapes, and regions. This type of social science inquiry requires thinking about what perspectives are present or absent in negotiations and decision-making and the potential options for and implications of actions based on complex power dynamics and inequalities (Scoones 1999).

Together, these 3 approaches form a multiparadigmatic and multimethod framework for assessing the human dimensions of mountain landscapes and linking mountain observatories in a global network. The framework shares similarities with the social impact assessment (SIA) approach (Vanclay et al 2015) and the driver pressure state impact response (DPSIR) framework (EEA 1999). While the SIA approach seeks to document multidimensional attributes, it is most often used for the evaluation of impacts associated with a particular development action (Esteves et al 2012), rather than the broader environmental actions and conditions that are the focus of mountain observatories. However, the SIA's well-developed community-profiling techniques, which assess local needs and aspirations, as well as key social issues, are valuable both as indicators and as community engagement methods and could be readily incorporated in mountain observatory efforts (Esteves et al 2012).

Designed to describe the origins and consequences of environmental problems, the DPSIR framework emphasizes stable indicators associated with environmental drivers, pressures, states, impacts, and responses but may be insufficient to capture trends over time or the power dynamics that often subjugate the interests and knowledge of local stakeholders (Carr et al 2007). Svarstad et al (2008) showed that the DPSIR framework is incompatible with various value orientations and perpetuates a barrier to greater stakeholder participation, which is necessary for robust assessments and observations of landscape conditions and dynamics. The framework outlined in this paper may combine well with the DPSIR framework to expand the range of considerations and perspectives incorporated into mountain observatories.

To fully achieve sustainable development goals, the perspectives and knowledge of nonscientific actors in mountain landscapes must also be integrated into mountain observatories (Kläy et al 2015). Participatory and engaged methods often incorporated by constructivist and critical social scientists help to incorporate more local, indigenous, or situated knowledge (Irwin 2001). As revealed by the survey of participants in the Perth III mountain conference (Gleeson et al 2016), the mountain research community appears to be well connected to societal partners: of more than 300 participants, nearly half (45%) rated their connection as 4 or 5 on a 5-point scale (1 = little interaction; 5 = abundant interaction). The transdisciplinary focus was higher for social scientists (68%) than for biophysical scientists (36%). These data suggest that social science members of the mountain research community can help expand engagement with knowledge holders beyond the scientific community (Gleeson et al 2016).

Conclusion

By organizing the GNOMO initiative for the pursuit of sustainable mountain development, the mountain research community has committed not only to interdisciplinary science but also to "actionable science" that informs decision-making, improves policies, and serves society (Palmer 2012). Such commitment requires breaking down paradigmatic differences not only between the social and the natural sciences but also within the social sciences. Furthermore, innovative participatory engagement methods are needed to reach beyond scientific perspectives to most fully observe mountain systems.

The framework highlighted in this paper suggests that the divergent paradigms within the social sciences can be embraced within a network of mountain observatories. This does not mean that each scientist must endeavor to put each paradigm into practice. Instead, by supporting research and observatory networks and committing to constructive dialogue among scientists, practitioners, decision-makers, and other stakeholders (Brown et al 2015), deeper integrative understanding is possible. Admittedly, this transparadigmatic reorientation of the GNOMO effort will require a philosophical shift by an international and multidisciplinary group of researchers. But there is precedent in other international research communities, such as the Millennium Ecosystem Assessment, the Earth System Science Partnership, and Future Earth (Mooney et al 2013). I hope we will seize this opportunity to build on these examples to create a more holistic and robust global network of mountain observatories by adopting an inclusive approach across and beyond sciences.

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REFERENCES

Björnsen Gurung A, Wymann von Dach S, Price MF, Aspinall R, Balsiger J, Baron JS, Sharma E, Greenwood G, Kohler T. 2012. Global change and the world's mountains: Research needs and emerging themes for sustainable development. *Mountain Research and Development* 32(S1):47–54.

Bliss JC. 1999. Understanding people in the landscape: Social research applications for ecological stewardship. *In:* Sexton WT, Malk AJ, Szaro RC, Johnson NC, editors. *Ecological Stewardship: A Common Reference for Ecosystem Management*. Vol. 3. Oxford, United Kingdom: Elsevier Science, pp 43–57.

Brown RR, Deletic A, Wong THF. 2015. Interdisciplinarity: How to catalyse collaboration. *Nature* 525(7569):315–317.

Carr ER, Wingard PM, Yorty SC, Thompson MC, Jensen NK, Roberson J. 2007. Applying DPSIR to sustainable development. *International Journal of Sustainable Development & World Ecology* 14:543–555.

Cutter SL, Boruff BJ, Shirley WL. 2003. Social vulnerability to environmental hazards. *Social Science Quarterly* 84(2):242–261.

Debarbieux B, Price MF. 2008. Representing mountains: From local and national to global common good. *Geopolitics* 13:148–168.

De Lange HJ, Sala S, Vighi M, Faber JH. 2010. Ecological vulnerability in risk assessment—A review and perspectives. *Science of the Total Environment* 408:3871–3879.

Eakin H, Luers AL. 2006. Assessing the vulnerability of social–environmental systems. *Annual Review of Environmental Resources* 31:365–394.

EEA [European Environment Agency]. 1999. *Environmental Indicators: Typology and Overview*. Technical report 25. Copenhagen, Denmark: EEA.

Esteves AM, Franks D, Vanclay F. 2012. Social impact assessment: The state of the art. *Impact Assessment and Project Appraisal* 31(1):34–42.

Flint CG, Kunze I, Muhar A, Yoshida Y, Penker M. 2013. Exploring empirical typologies of human–nature relationships and linkages to the ecosystem services concept. *Landscape and Urban Planning* 120:208–217.

Freudenburg WR. 1996. Strange chemistry: Environmental risk conflicts in a world of science, values, and blind spots. *In:* Cothern CR, editor. *Handbook for Environmental Risk Decision Making: Values, Perceptions, and Ethics*. Boca Raton, FL: CRC, pp 11–36.

Freudenburg WR, Frickel S, Gramling R. 1995. Beyond the nature/society divide: Learning to think about a mountain. *Sociological Forum* 10(3):361–392.
Future Earth. 2014. *Future Earth Strategic Research Agenda*. Paris, France: International Council for Science.
Geertz C. 2000. *Local Knowledge*. New York, NY: Basic Books.
Gleeson EH, Wymann von Dach S, Flint CG, Greenwood GB, Price MF, Balsiger J, Nolin A, Vanacker V. 2016. Mountains of our future earth: Defining priorities for mountain research—A synthesis from the 2015 Perth III conference. *Mountain Research and Development* 36(4):537–548.
Gómez-Baggethun E, de Groot R. 2010. Natural capital and ecosystem services: The ecological foundation of human society. *Issues in Environmental Science and Technology* 30:105–121.
Greene JC, Caracelli VJ. 2003. Making paradigmatic sense of mixed methods practice. *In:* Tashakkori A, Teddlie C, editors. *Handbook of Mixed Methods in Social and Behavioral Research*. Thousand Oaks, CA: Sage, pp 91–110.
Greenwood G. 2013. Mountain Research Initiative seeks to break new ground in second decade. *Mountain Research and Development* 33(4):473–476.
Grêt-Regamey A, Brunner SH, Kienast F. 2012. Mountain ecosystem services: Who cares? *Mountain Research and Development* 32(S1):S23–S34.
Holmberg J, Lundqvist U, Robèrt K, Wackernagel M. 1999. The ecological footprint from a systems perspective of sustainability. *International Journal of Sustainable Development & World Ecology* 6(1):17–33.
Irwin A. 2001. *Sociology and the Environment*. Cambridge, United Kingdom: Polity.
Kinzig A. 2001. Bridging disciplinary divides to address environmental and intellectual challenges. *Ecosystems* 4:709–715.
Kläy A, Zimmermann AB, Schneider F. 2015. Rethinking science for sustainable development: Reflexive interaction for a paradigm transformation. *Futures* 65:72–85.
Kumar C. 2005. Revisiting "community" in community-based natural resource management. *Community Development Journal* 40(3):275–285.
Larson EC, Luloff AE, Bridger JC, Brennan MA. 2015. Community as a mechanism for transcending wellbeing at the individual, social, and ecological levels. *Community Development* 4:407–419.
Lassoie JP, Sherman RE. 2010. Promoting a coupled human and natural systems approach to addressing conservation in complex mountainous landscapes of Central Asia. *Frontiers of Earth Science in China* 4(1):67–82.
Leiserowitz AA, Kates RW, Parris TM. 2006. Sustainability values, attitudes, and behaviors: A review of multinational and global trends. *Annual Review of Environment and Resources* 31:413–44.
MacMynowski DP. 2009. Pausing at the brink of interdisciplinarity: Power and knowledge at the meeting of social and biophysical science. *Ecology & Society* 12:20.
Messer NC, Jagai JS, Rappazzo KM, Lobdell DT. 2014. Construction of an environmental quality index for public health research. *Environmental Health* 13:39.
Messerli B. 2012. Global change and the world's mountains. *Mountain Research and Development* 32(S1):S55–S63.
Messerli B, Ives JD. 1997. *Mountains of the World: A Global Priority*. New York, NY: Parthenon.
Mooney HA, Duraiappah A, Larigauderi A. 2013. Evolution of natural and social science interactions in global change research programs. *PNAS* 110:3665–3672.
Neuman, WL. 2006. *Social Research Methods*. Boston, MA: Pearson.
OECD [Organisation for Economic Co-operation and Development]. 2016. Better Life Index. www.oecdbetterlifeindex.org; accessed on 15 September 2016.
Ostrom E. 2009. A general framework for analyzing sustainability of social–ecological systems. *Science* 325:419–422.
Ostrom E. 2011. Background on the institutional analysis and development framework. *Policy Studies Journal* 39(1):7–27.
Palmer MA. 2012. Socioenvironmental sustainability and actionable science. *BioScience* 62(1):5–6.
Panos Oral Testimony Programme. n.d. Mountain Voices. www.mountainvoices.org; accessed on 30 October 2015.
Peralvo M, Bustamante M. 2014. Implementing long-term monitoring platforms of coupled social–environmental dynamics in mountain ecosystems. Unpublished synthesis report of the Global Fair and Workshop on Long-Term Observatories of Mountain Social–Ecological Systems, Reno, Nevada, 16–19 July 2014. Available from author of this article.
Pohl C, Hirsch Hadorn G. 2007. *Principles for Designing Transdisciplinary Research*. Munich, Germany: Oekom Verlag.
Price LW. 1986. *Mountains and Man: A Study of Process and Environment*. Berkeley, CA: University of California Press.
Price MF, Byers AC, Friend DA, Kohler T, Price LW. 2013. *Mountain Geography: Physical and Human Dimensions*. Berkeley, CA: University of California Press.
Prosperi P, Allen T, Padilla M, Peri I, Cogill B. 2014. Sustainability and food & nutrition security: A vulnerability assessment framework for the Mediterranean Region. *SAGE Open* April–June:1–15. http://dx.doi.org/10.1177/2158244014539169; accessed on 15 September 2016.
Robbins P. 2011. *Political Ecology*. 2nd edition. Somerset, NJ: John Wiley.
Scoones I. 1999. New ecology and the social sciences: What prospects for a fruitful engagement? *Annual Review of Anthropology* 28:479–507.
Strang V. 2009. Integrating the social and natural sciences in environmental research: A discussion paper. *Environment, Development and Sustainability* 11:1–18.
Summers JK, Smith LM, Harwell LC, Case JL, Wade CM, Staub KR, Smith HM. 2014. An index of human well-being for the U.S.: A TRIO approach. *Sustainability* 6:3915–3935.
Svarstad H, Petersen LK, Rothman D, Siepel H, Wätzold F. 2008. Discursive biases of the environmental research framework DPSIR. *Land Use Policy* 25:116–125.
Thomas WI, Thomas DS. 1928. *The Child in America*: *Behavior Problems and Programs*. New York, NY: Knopf.
UN [United Nations]. 2015. *Transforming our World: The 2030 Agenda for Sustainable Development*. A/RES/70/1. New York, NY: UN.
UNCED [United Nations Conference on Environment and Development]. 1992. *Agenda 21, Rio Declaration, Forest Principles*. New York, NY: UN.
UNDP [United Nations Development Programme]. 2016. *Human Development Index*. http://hdr.undp.org/en/content/human-development-index-hdi; accessed on 15 September 2016.
Vanclay F, Esteves AM, Aucamp I, Franks D. 2015. *Social Impact Assessment: Guidance for Assessing and Managing the Social Impacts of Projects*. Fargo ND: International Association for Impact Assessment.
Wallerstein IM. 1991. *Unthinking Social Science: The Limits of Nineteenth-Century Paradigms*. Philadelphia, PA: Temple University Press.
Westley F, Carpenter SR, Brock WA, Holling CS, Gunderson LH. 2001. Why systems of people and nature are not just social and ecological systems. *In:* Gunderson LH, Holling CS, editors. *Panarchy: Understanding Transformations in Human and Natural Systems*. Washington, DC: Island Press, pp 103–119.
Wilkinson K. 1991. *The Community in Rural America*. Westport, CT: Greenwood.
Williams DR. 2014. Making sense of "place": Reflections on pluralism and positionality in place research. *Landscape and Urban Planning* 131:74–82.
Wu J. 2006. Landscape ecology, cross-disciplinarity, and sustainability science. *Landscape Ecology* 21:1–4.

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THEME SECTION PAPER

Multi-paradigm modelling for cyber–physical systems: a descriptive framework

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Abstract

The complexity of cyber–physical systems (CPSs) is commonly addressed through complex *workflows*, involving models in a plethora of different *formalisms*, each with their own methods, techniques, and tools. Some *workflow patterns*, combined with particular *types of formalisms* and *operations* on models in these formalisms, are used successfully in engineering practice. To identify and reuse them, we refer to these combinations of workflow and formalism patterns as modelling *paradigms*. This paper proposes a *unifying (Descriptive) Framework* to describe these paradigms, as well as their combinations. This work is set in the context of Multi-Paradigm Modelling *(*MPM), which is based on the principle to model every part and aspect of a system explicitly, at the most appropriate level(s) of abstraction, using the most appropriate modelling formalism(s) and workflows. The purpose of the Descriptive Framework presented in this paper is to serve as a basis to reason about these formalisms, workflows, and their combinations. One crucial part of the framework is the ability to capture the *structural* essence of a paradigm through the concept of a *paradigmatic structure*. This is illustrated informally by means of two example paradigms commonly used in CPS: Discrete Event Dynamic Systems and Synchronous Data Flow. The presented framework also identifies the need to establish whether a paradigm *candidate* follows, or qualifies as, a (given) paradigm. To illustrate the ability of the framework to support *combining* paradigms, the paper shows examples of both workflow and formalism combinations. The presented framework is intended as a basis for characterisation and classification of paradigms, as a starting point for a rigorous formalisation of the framework (allowing formal analyses), and as a foundation for MPM tool development.

Keywords Multi-paradigm modelling · Foundations of model-based systems engineering · Cyber–physical systems

1 Introduction

Cyber–Physical Systems (CPSs) are engineered systems that emerge from the networking of multi-physical processes (mechanical, electrical, biochemical, etc.) and computational

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processes (control, signal processing, logical inference, planning, etc.) that typically interact with a highly uncertain environment, including human actors, in a socio-economic context. These systems enable many of our daily activities and have become innovation drivers in important domains, such as automotive, avionics, civil engineering, Industry 4.0, and robotics.

Engineering CPSs requires the contribution of experts from different domains to solve the challenges related to their own discipline, but also to collaborate to make all parts work together. Because CPSs are generally costly to fully build and maintain, early modelling and simulation is a de facto technique crucial in their development. This enables reconciling the multifaceted aspects of a CPS, studying safety-critical and emerging properties, and planning for deployment even before the physical parts of the system are available (e.g. via Hardware-in-the-Loop (HIL) simulation).

The full complexity of CPS engineering is not covered by single modelling paradigms. For instance, the Equation-Based paradigm only covers the physical parts of the system; the Object-oriented paradigm only covers the code parts of the system; and the Agile paradigm only covers workflow aspects of system development. Consequently, the heterogeneity and complexity of CPSs and their design activities require the combination of multiple paradigms to describe the entire system while including all relevant aspects.

In this context, what is a *paradigm* then? The science philosopher Kuhn defines it as "an open-ended contribution that frames the thinking of an object study with concepts, results and procedures that structures future achievements" [42]. Though seemingly far from the concerns in the discipline of computer science, this definition does highlight the emergence of a *structure* that captures the object of discourse and the existence of *procedure*s that guides achievements.

In computer science, paradigms are probably best known as a means for classifying General-purpose Programming Languages (GPLs). For example, Eiffel is Object-Oriented and supports Contract-Based Design, Prolog is considered Declarative, while Lisp is Functional. A paradigm characterises both the syntax *and* semantics of the language including principles that govern it: Object Orientation imposes viewing the world in terms of communicating objects typed by classes, whereas the declarative paradigm relies on term substitution and rewriting. The idea of combining several paradigms into a single GPL led to more expressive, powerful programming languages such as Java [28] (which is Imperative, Object-Oriented, Concurrent, Real-Time, and Functional) and Maude [13] (which is Declarative, Object-Oriented, Concurrent, and Real-Time), among many others.

Multi-Paradigm Modelling (MPM) has only recently been recognized as a powerful paradigm on its own that can help to design, as well as communicate and reason about, CPSs. The term MPM finds its origin in the Modelling and Simulation community in 1996, when the EU ESPRIT Basic Research Working Group 8467 "Simulation in Europe" (SiE) formulated a collection of research directions and policy guidelines [69] identifying the need for "a multi-paradigm methodology to express model knowledge using a blend of different abstract representations rather than inventing some new super-paradigm". The main result was a vision where all parts and aspects of a complex system are modelled explicitly, using the most appropriate modelling formalisms to deal with engineering heterogeneity. The important aspect of workflow was not yet present. At first, only problems were identified, but later on, the same group focused on combining multiple formalisms [70] through architectural composition (as opposed to view composition). One main merit of the SiE work was the inclusion of **a-causal** modelling to model physical phenomena, an effort that led to the design of the Modelica language.

Physical systems are often modelled using continuous abstractions, e.g. Differential Algebraic Equations (DAEs) to express constituent equations relating physical variables of interest. Software systems are often modelled using discrete abstractions, e.g. State Automata to express the discrete changes made to data stored in memory by executing program instructions. A consequence of the fact that CPSs combine cyber (software) and physical components is that they are naturally modelled using *hybrid* modelling languages that combine continuous and discrete abstractions [79]. The meaningful and usable integration of discrete and continuous domains is at the heart of dealing with CPS. More generally, dealing with heterogeneity, both in the levels of abstraction and in the formalisms used, is one of the major challenges in modelling CPSs.

The main contribution of this paper is a Descriptive Framework for MPM applied to CPSs. The framework is based on a special kind of metamodel where *placeholders* can be used, capturing various *structural* and *process* patterns. Such metamodels support expressing property expressions that we call *paradigmatic* properties: they are used to capture the essence of a paradigm and can be bound to existing elements of candidate formalism/workflow metamodels (as well as their semantics) to determine if the candidate formalism(s)/workflow(s) effectively follow the paradigm.

Although not completely formal, our framework allows experts to better grasp the essence of how their CPSs are designed, while providing a common ground for a rigorous engineering of CPSs based on their MPM components. Ultimately, in a next step not covered by this paper, this framework aims to support tool builders, language developers, analysis engineers and other experts to reason about CPSs and figure out which formalisms, abstractions, workflows and supporting methods, techniques, and tools are the *most appropriate* to carry out their task(s), thus minimising accidental complexity due to non-optimal **tool** selection. Note that this paper does not intend to present a classification of formalisms or workflows that could be used to engineer CPSs. However, our Descriptive Framework could be used to better classify these elements by providing more precise descriptions for them.

This paper is a continuation of an effort started during the COST Action IC1404[1] "Multi-Paradigm Modelling for Cyber-Physical Systems" (MPM4CPS), which surveyed languages and tools used for engineering CPSs [12] and captured the relationships between them in an ontology. Moreover, it significantly extends, and complements, a preliminary version of our Descriptive Framework [3] by (i) capturing the various components of a paradigm explicitly and (ii) demonstrating a simple paradigm *combination* resulting in a valid paradigm, which could suggest that our framework is closed under the usual combination operators required for the *multi*-paradigms necessary for modelling CPSs.

We organised the paper as follows. Section 2 presents an informal notion of paradigm to serve as a tutorial introduction to our Descriptive Framework, which itself is described in Sect. 3. Section 4 exemplifies the framework with two well-known paradigms used for CPS development. Section 5 defines a paradigm combinator, namely *embedding*, and shows how to systematically build a paradigm candidate from candidates of the combined paradigms. Section 6 highlights and discusses related work from other communities, and Sect. 7 reflects on our results. Section 8 proposes future lines of research and concluding remarks.

2 What is a paradigm?

Broadly speaking, a *paradigm* acts as a *pattern* for describing a whole class of artefacts sharing similar characteristics or designates a framework that encapsulates theories inside a scientific domain. We aim to capture the meaning of the paradigm concept precisely enough to make it ultimately amenable to computer-based analysis and reasoning.

This section provides an intuitive and lightweight introduction to what a paradigm is. We start by a small detour in linguistics and epistemology to revisit the classical definitions in these fields, before focusing again on their meaning in computer science. Using two well-known paradigm examples from computer science, namely the Object Orientation and *Agile development* paradigms, we clarify the core components of our Descriptive Framework. The structure of this framework is then described by means of a metamodel and illustrated through typical usage scenarios.

[1] http://mpm4cps.eu.

2.1 General definitions

From a *linguistic* viewpoint, a *paradigm* has three definitions from the English dictionary:

- A *framework* containing basic assumptions, ways of thinking, and methodology that are commonly accepted by members of a scientific community [57];
- A philosophical and theoretical framework of a scientific school [of thought] or discipline within which are formulated theories, laws, and generalisations, as well as the experiments performed in support of [53].
- A model of something, or a very clear and typical *example* of something [11].

Although very general in nature, there are several aspects of these linguistic definitions that are worth pointing out. First, in each of the above definitions, a paradigm defines, in some sense, a *structure* that is shared by several elements the paradigm is intended to capture. Second, a paradigm also provides a way of *deciding* whether an element under analysis possesses those "basic assumptions" for fitting the structure. Third, a paradigm organises the elements it characterises in such a way that it becomes possible to *reason* about them (with the help of "theories", "laws" and suitable "generalisations"). Finally, a paradigm results from an *agreement* between "members of a [scientific] community": the precise definition may change over time and may be slightly different from different "schools of thought", though sharing "basic assumptions".

In the field of philosophy of science, the most popular and commonly agreed-upon definition of the concept of paradigm was formulated by Kuhn [42], who distinguishes the following:

- The subject matter, i.e. what is to be observed and scrutinised;
- The kind of questions that are supposed to be asked and probed for answers in relation to the subject;
- How these questions are to be structured;
- What predictions are made by the primary theory within the discipline;
- How the results of scientific investigations should be interpreted;
- How an experiment is to be conducted and which equipment is available to conduct these experiments.

The aspects highlighted by this philosophical definition are similar to the linguistic ones pointed out above, although differently framed. Kuhn gives some details about how the reasoning takes place: he emphasises that a paradigm is *questioned* in a *structured* way, and that some of these questions may be general enough to form the basis of predictions about the subject matter.

Let us summarise what we learnt about the nature and functions of a paradigm:

1. A paradigm captures the *essence* of a collection of elements that have a substantial impact in a scientific discipline.
2. As a consequence, a paradigm is ontologically *distinct* from those elements.
3. The essence captured by a paradigm is expressed through "questions" or, in the case of computer science, *properties of interest* that are supported by various *structures*.
4. Those properties enable *reasoning* and *drawing suitable generalisations*, and *predictions*. They also offer a way of *deciding* whether an element of interest (that we later call a "*candidate*") *qualifies as*, *follows*, or *embodies* this paradigm, typically by human assessment.

We claim that in computer science, the "questions" for a paradigm, or *paradigmatic properties* as we will call them, always rely on structures that are supported by *processes*, or *workflows*, for capturing the dynamic nature of computations, processes that ultimately manipulate *formalisms*.

In the next section, we purposely study two paradigm examples (in a simplified version) that are widely recognised as having significantly shifted the scientific field of computer science, namely Object Orientation and Agile Programming. Note that these are programming paradigms, which constitute a specific subclass of modelling paradigms, with the advantage of being readily understood by readers from the Software Engineering community. Both are chosen on purpose: the former pertains to formalisms, whereas the latter pertains to processes.

For the purpose of the presentation, we had to choose a particular way of describing those concepts using *supportive formalisms* (which correspond to meta-metamodels, or technical spaces, see Wimmer and Kramler [77]). Note, however, that our Descriptive Framework does not depend on any particular choice of supportive formalism(s): only the expression of the (paradigmatic) properties and their underlying structures depend on them for reasoning and deciding whether a (candidate) element follows a given paradigm. We further discuss this point at the end of each example.

2.2 Two simple examples: Object Orientation and Agile Programming

An important feature for paradigms, which is crucial to clarify the discourse, is the ability to explicitly *name* both the properties a paradigm relies on, and as well as variations of a paradigm. We present in this section two (versions of) well-known paradigms in computer science and discuss some of their characteristic properties. For each paradigm p, we adopt a similar presentation:

1. We provide background information on paradigm p to point out why it significantly impacted programming;
2. We focus on *one* singular property π of p that is common enough to make it easy to grasp, and simple enough to be easily demonstrated without introducing too much notation;
3. We present two *candidate* elements $\mathcal{C}1$ and $\mathcal{C}2$, one for which π is satisfied, and the other for which it is not;
4. We list the required *supporting formalisms* necessary for building our Descriptive Framework and illustrate them on the basis of our candidates.

2.2.1 Object Orientation: a formalism-oriented paradigm

Object Orientation (OO) emerged in the 1960s in response to a need to structure the way programs were specified. Instead of seeing a computation as just imperative processing of sequential instructions, OO defines and structures computation through organised, communicating objects that are typed by means of classes, which define their structure as well as their computation and communication capabilities. OO concepts are applicable in software engineering sub-domains such as analysis, design, and software development. Whether a GPL is classified as OO depends on how tightly integrated the OO concepts are into the programming language: from "pure" OO GPLs where every programming construct is an object (e.g. in Eiffel or Scala), over GPLs that still contain some procedural elements (e.g. Java or C), to GPLs that integrate some specific concepts (e.g. Ada or MATLAB).

There exist many variations of the definition of the OO paradigm for GPLs (cf. among others, [1,75]). As a possible classification, Wegner [75] distinguishes the notions of object-based and object-oriented GPLs that may support (or fail to support) data abstraction, strong typing, and delegation. For illustrative purposes, let us only consider a very basic feature, namely *inheritance*, as a language mechanism to share and factor out properties, thus promoting reuse. When a (sub-)class C inherits from a (super-)class C', then semantically, all objects that are instances of C automatically inherit the state and behaviour of C'. Of course, many other more complex properties define the OO paradigm, and potentially several variations of the same property (e.g. allowing *multiple* inheritance) may be considered. As described previously, a paradigm is often an agreement or a common understanding in a scientific school of thought, but nothing prevents the co-existence of several variations of definitions that are similar. Discriminating between them may be achieved through distinct *names* relating to different (variations of) the set of properties that characterise a given paradigm.

One may be interested in checking that a given *candidate* GPL actually qualifies as OO. Let us consider Java [28] and Pascal [15] for the purpose of the discussion. For doing so, one needs to check whether the properties defining (the particular flavour of) OO are indeed satisfied by such a candidate GPL. Note that a given candidate GPL is itself a language specified with candidate formalisms: one for capturing its concrete syntax the programmer manipulates and one for providing executability through an operational and/or a translational semantics. We will qualify those as *candidate* formalisms, to distinguish them from the *paradigmatic* formalisms used for capturing the specifics of a given paradigm.

Completely formalising those properties still requires the use of appropriate *supporting* formalisms for capturing them and a way to relate the descriptions to the formalisms defining the candidates, to check the properties' satisfaction.

To summarise, we considered the paradigm p as being Object Orientation, for which one of the characteristic properties π is *inheritance*, with two potential candidate elements $\mathcal{C}1$ as Java, and $\mathcal{C}2$ as Pascal. To be able to actually check whether $\mathcal{C}1$ and $\mathcal{C}2$ qualify as Object Oriented, we need at least four kinds of formalisms:

1. A *structural* (paradigmatic) formalism for describing structures, to name, organise and relate the concepts required by the paradigm. In the case of *inheritance*, this (paradigmatic) formalism would capture the notions of class, fields and objects and their relationships, as described, e.g. by Wegner [75]. Depending on the properties of interest characterising a given paradigm, this (paradigmatic) formalism may be used to capture patterns at both the *syntactic* and *semantic* level of a candidate, since paradigmatic properties often concern both (as it is the case for the inheritance property described earlier anyway).
   Figure 1 (top) illustrates one way to capture the structure necessary for expressing the inheritance property using a Placeholder Class Diagram inspired by the UML MOF syntax (where placeholders are represented as double rectangle "classes").
2. In the context of GPLs, candidates are usually already existing programming languages, defined in a given (candidate) formalism. Java and Pascal certainly have a BNF grammar definition historically, and Java may have a UML Class Diagram-based (e.g. as a metamodel in the Eclipse platform) or a Graph Grammar-based definition (e.g. Corradini et al. [16], among others).
   Figure 1 (bottom) represents the (simplified) metamodels of two GPLs, Java and Pascal, as *candidates* for the OO paradigm, using a MOF Class Diagram.
3. A *mapping* formalism for relating the structural (paradigmatic) formalism with the candidate formalisms. This mapping is essential because the patterns captured by the paradigm p need to be related to specific (sub-)structures in the candidates. Precisely defining this mapping formalism is out of the scope of this paper; we explain only informally how this mapping would occur (or fail to) for our candidates Java and Pascal.
   We need to check whether the topological structure from Fig. 1 may be matched against both GPLs' metamodels and if so, whether the property is satisfied (modulo the matching) on the corresponding structures.
   A Pascal Program is composed of Blocks, which are either constant, variable, or type definitions, or alternatively function and procedure declarations. None of these concepts would fully match against the C placeholder, because no association can be appropriately matched against the super reflexive association, nor with an appropriate match with VF and its own associations. Without further analysis, one can confidently conclude that Pascal does not qualify as OO.
   In the Java metamodel, however, the NormalClassDeclaration is a good candidate for a match with the C placeholder, since it also contains ClassMemberDeclarations where FieldDeclarations may potentially match the TF placeholder, with the super relationship being expressed with extends (as the textual representation of super in the left of Fig. 1). Notice that Java is actually richer: interfaces may also match with C, but would fail for the rest (since Java's interfaces do not declare fields); and Java allows field overloading.
4. Finally, a *property* (paradigmatic) formalism for specifying properties over the structural (paradigmatic) formalism, as well as an appropriate checking procedure allowing to validate, via the mapping, that a candidate GPL satisfies the expressed (paradigmatic) properties. Following our choice of Placeholder Class Diagram as a structural paradigmatic formalism, a natural choice for expressing our inheritance property would leverage the OCL language that could accommodate with placeholders. Again, without going into too much formal specification, we rely on the usual OCL syntax to try and express inheritance, in two steps.
   First, the set of accessible fields for an object is recursively computed by climbing up the super relationship in the object's typing class.

```
context O inv valuedFieldsMatchAccessibleFields :
    let valFieldNames : Set(String) =
        o.valFields.name
    in o.type.accessibleFields()
        ->collect(tf | tf.name)-> forAll(tfName |
            valFieldNames.exists(tfName))
```

Since Pascal presented no match for the structural patterns of the *inheritance* property, there is no need to try and check the property itself. For the Java case,

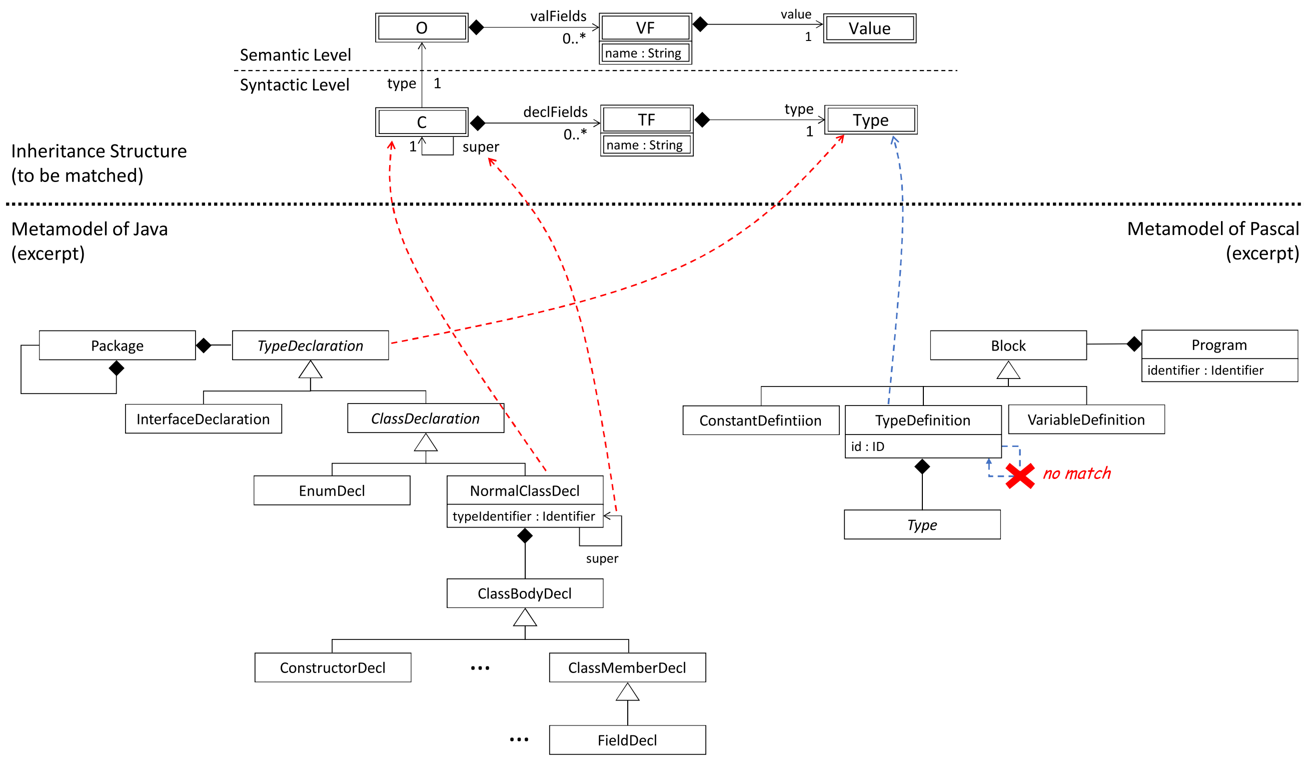


Fig. 1 On top, an example of a Placeholder Class Diagram for capturing concepts and relationships needed for expressing paradigmatic properties, using a UML MOF-based syntax: "placeholder" classes are depicted with double rectangles (instead of the regular rectangles for UML Class Diagram), to indicate that classes are meant to be matched into a candidate metamodel. The example illustrates (part of) the *inheritance* property of the OO paradigm. On the left, an excerpt of a metamodel for the Java GPL, and one for the Pascal GPL on the right, showing how (syntactic) may be appropriately matched or not

the nature of *inheritance* requires to have a look at the semantic level to check for a similar mechanism. Stärk et al. [61] proposed a formal semantics for Java based on Abstract State Machines, which are directly executable, and compared their specification with the Java Compiler. Their specification defines (algebraic) functions for class (namely $classFieldValues$) and instance field ($instFieldValue$) declarations, and models the dynamic state of objects through their reference; both collect the so-called *accessible* fields for an object and are updated with the semantic rules translating the effect of field access and assignment. The Inheritance property π is enforced in their semantic specification by simply ensuring that the (algebraic) total functions share appropriate domains (thus forcing accessible fields to possess a value, be it the value used at initialisation).

A formal proof is obviously out of this paper's scope, but this simple example already demonstrates how it may be difficult to relate and check properties expressed in different supporting formalisms (an OCL-like expression for the paradigmatic property and an algebraic expression for the Java candidate).

2.2.2 Agile development: a workflow-oriented paradigm

Agile development (AD) emerged in the early 2000s as an alternative to the so-called heavyweight software development processes (such as the traditional V-model), because many software development projects required less regulation, a shorter response time to requirement changes from customers during the course of a project, and the processes were perceived as overly constraining for developers, hampering creativity. The general principles of AD were summarised in the Agile Manifesto [50], a general guide that places people and software deliverables at the centre of the software development process, rather than more rigid and procedural processes that may lose the final objective of delivering high-quality software out of sight.

Here again, multiple variations for the definition of the AD paradigm as a software development process exist (cf. Merkow [52], Przybyłek and Morales–Trujillo [59], among others). A key feature of AD that distinguishes it from classical software development approaches is its iterative nature. Organising shorter "full cycle" phases (from requirements to delivered software), in each of which a smaller set of requirements are addressed, actually helps both parties: the stakeholders gain confidence in the developed software, which enables them to express their needs more precisely, while the developers deliver solid, well-tested pieces of the final product, responding quickly to new insights and updated needs. Selecting a feasible set of functionalities is crucial for the success of the so-called sprint phases: it is because the tasks are voluntarily reduced to covering meaningful, small increments in functionality, that it becomes possible to achieve a "full cycle" in a limited time.

For illustrative purposes, let us consider a generic Design activity that performs what is considered as a "full cycle" or Sprint. For each Sprint, a limited set of requirements needs to be selected from the complete set of requirement, thus capturing the stakeholders' priorities. The selected set must be small enough such that the sprint can be performed in a reasonable short time. Some variants of AD even require fixed-length sprints. At the end of the sprint, an assessment of the maturity of the requirements' fulfilment is performed, leading to a new evaluation of the priorities, thus entering a new sprint.

To formalise the key features of AD, one needs the means to again manipulate concepts at both the *syntactic* and *semantic* levels. Syntactically, we need to describe the notion of "activity" that takes as input (a subset of) the requirements, expressed in an appropriate formalism; and the control flow associated with the loop enclosing a sprint. Semantically, we need to ensure that any sprint execution is performed within some time limit.

In summary, in order to precisely formalise our paradigm P of choice, in this case, Agile Development, for which one characteristic property π is the fact that a sprint is performed in a reasonably short time, we consider two potential candidate elements $\mathcal{C}_1$, being the (simplified) SystemDesignPhase of the V-model, and $\mathcal{C}_2$, being a (simplified form of) SystemDesignExploration. For checking whether $\mathcal{C}_1$ and $\mathcal{C}_2$ qualify as agile development, we would need at least four kinds of formalisms:

1. A *structural* (paradigmatic) formalism for describing a *workflow* that enables distinguishing between control and artefact flows. Depending on the properties of interest characterising a given paradigm, this (paradigmatic) formalism may be used to capture patterns at both the syntactic and semantic level (i.e. over the execution traces of the paradigmatic workflow), since paradigmatic properties often concern both (as it is, for example, for the requirement that Agile loops span over short periods.

   Figure 2 (middle) depicts the (paradigmatic, structural) workflow associated with the AD key features using a UML Activity Diagram-like (our choice for the structural paradigmatic formalism listed above): the short ShortDesignActivity, contained in the Sprint activity, is a placeholder activity (note double-rounded rectangle used as a symbol, in contrast to the regular rounded rectangle in in UML Activity Diagrams)
2. In the context of Workflow specifications (cf. discussions in Sect. 6.4), candidates are usually already expressed in a given formalism. We sketch in Fig. 2 (top and bottom) (simplified versions of) parts of the V-Model development lifecycle and DesignSpaceExploration. We also use UML Activity Diagrams as a formalism to simplify the description.

   The upper part of Fig. 2 depicts a (simplified) SystemDesignPhase of the V-Model, with only requirements analysis and design activities shown (it is assumed that the design artefacts produced are executable and have been tested).
3. A *mapping* (paradigmatic) formalism for relating the structural (paradigmatic) formalism elements with a candidate formalism used for specifying the abstract syntax of potential candidate workflows: BPMN, UML Activity Diagrams, etc. Precisely defining this mapping formalism is out of this paper's scope; we only informally visualise it through the red dashed lines in Fig. 2.

   Although initially, a match of the SystemDesignPhase AD candidate seems possible (the dashed mapping arrows), it soon becomes obvious that the mapping cannot be completed as no control loop can be found in the SystemDesignPhase AD candidate. This comes as no surprise, as the essence of the V-model and its phases is its linear arrangement of activities. One may thus conclude that the V-Model's SystemDesignPhase does not qualify as Agile, since not even the syntactic components match.

   Consider now a multi-objective SystemDesignExploration process where many variants of a CPS may be explored, thus eliminating poor designs and keeping the ones that satisfy a set of global constraints to be further analysed against non-functional criteria such as performance, cost, power consumption, etc [48]. As the Agile *pattern* leaves the ShortDesignActivity unspecified, it will match any workflow candidate which contains, in the place of the ShortDesignActivity, a workflow that matches this activity's interface, and whose execution time qualifies as "short". As shown in Fig. 2, *substituting* a DesignSpaceExploration (DSE) workflow while respecting the appropriate "interface" for ShortDesignActivity guarantees acceptance as following AD.
4. A *property* (paradigmatic) formalism for specifying *properties* over the structural (paradigmatic) workflow, as well as an appropriate checking procedure to validate, via the mapping, that a candidate workflow satisfies the (paradigmatic) properties.

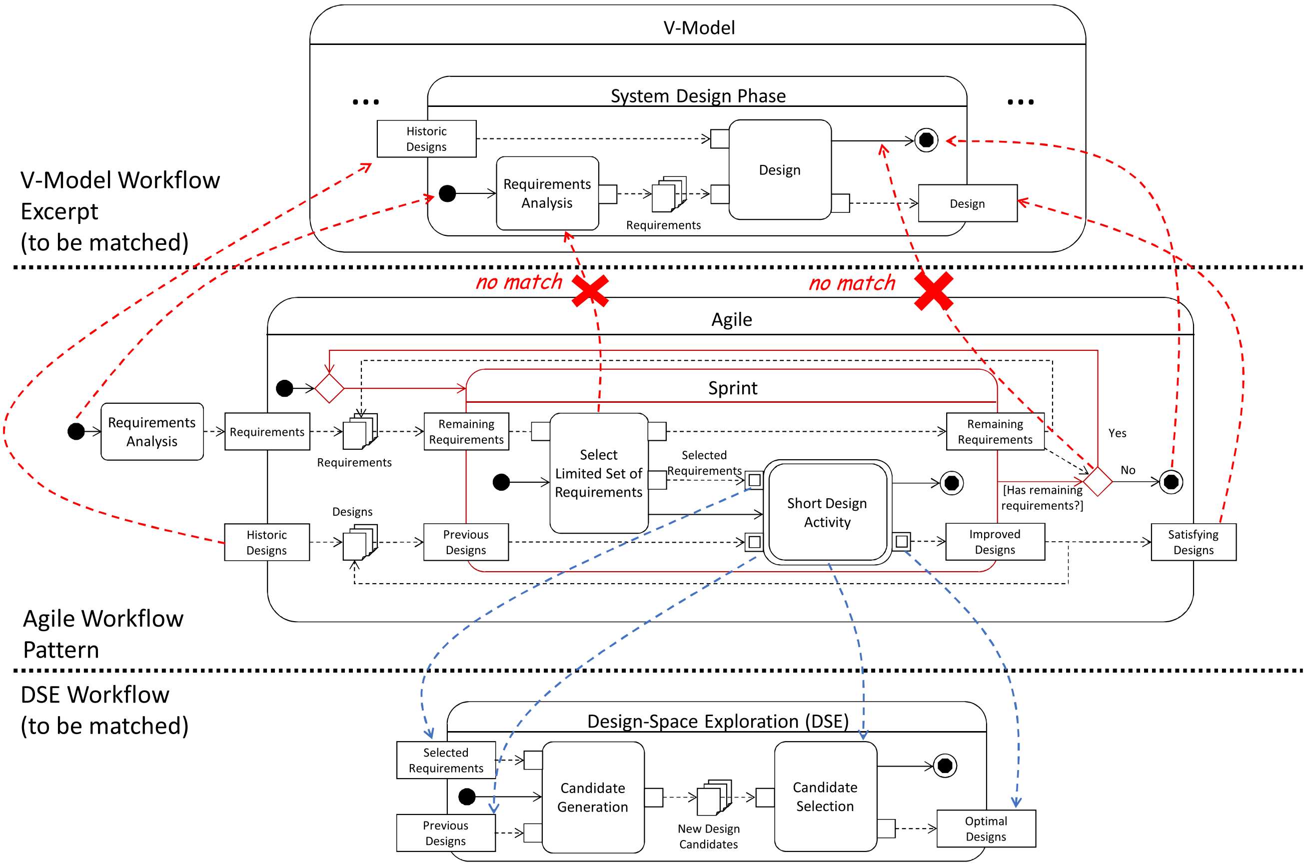


Fig. 2 A proposal for capturing the Agile development (AD) life cycle pattern, as a WorkflowPH in the middle. On the top, a representation of the SystemDesignPhase of the V-Model, which fails to fully match the AD pattern. The V-Model workflow essentially lacks a loop (so-called Sprint) that addresses a small, self-contained subset of requirements (it actually aims at the full set). On the bottom, a successful match between the AD workflow pattern and SystemDesignExploration if the latter is embedded in ShortDesignActivity

We would have to define a paradigmatic property for π in a formalism that would allow constraining the (potentially parameterisable) duration of the placeholder activity ShortDesignActivity in the Agile workflow pattern. Note that this property refers to the *trace semantics* of the structural paradigmatic formalism.

Design Space Exploration may in itself be characterised as a paradigm on its own, since it describes a characteristic way of producing valid, optimal designs that satisfy a selection of requirements. The use of patterns within the structural (paradigmatic) formalism (based here on UML Activity Diagrams) allows to easily describe *Agile* Design Space Exploration compositionally by separating the workflow for the Design Space Exploration paradigm from the one specifying its Agile nature. This leads to the notion of the proper combination of multiple paradigms: we further investigate one possible combination operator in Sect. 5.

3 A Descriptive Framework for capturing modelling paradigms

The complexity of (designing) CPSs is commonly addressed through complex *workflows*, involving models in a plethora of different *formalisms*, each with their own methods, techniques and tools, and combining particular *types of formalisms* and *operations* on models in these formalisms. MPM proposes to model everything explicitly, at the most appropriate level of abstraction, using the most appropriate modelling formalisms.

In the previous section, we offered a tutorial presentation and example of each constitutive element of a paradigm, as well as the intuition behind how to check whether a candidate qualifies as a paradigm's element: object orientation illustrated the *formalism* aspect with Java and Pascal as candidates. Agile development focused on the *workflow* aspect, with classical V-model and design space exploration life cycles. In this section, we go one step further and capture precisely, through a metamodel, the structuring elements of

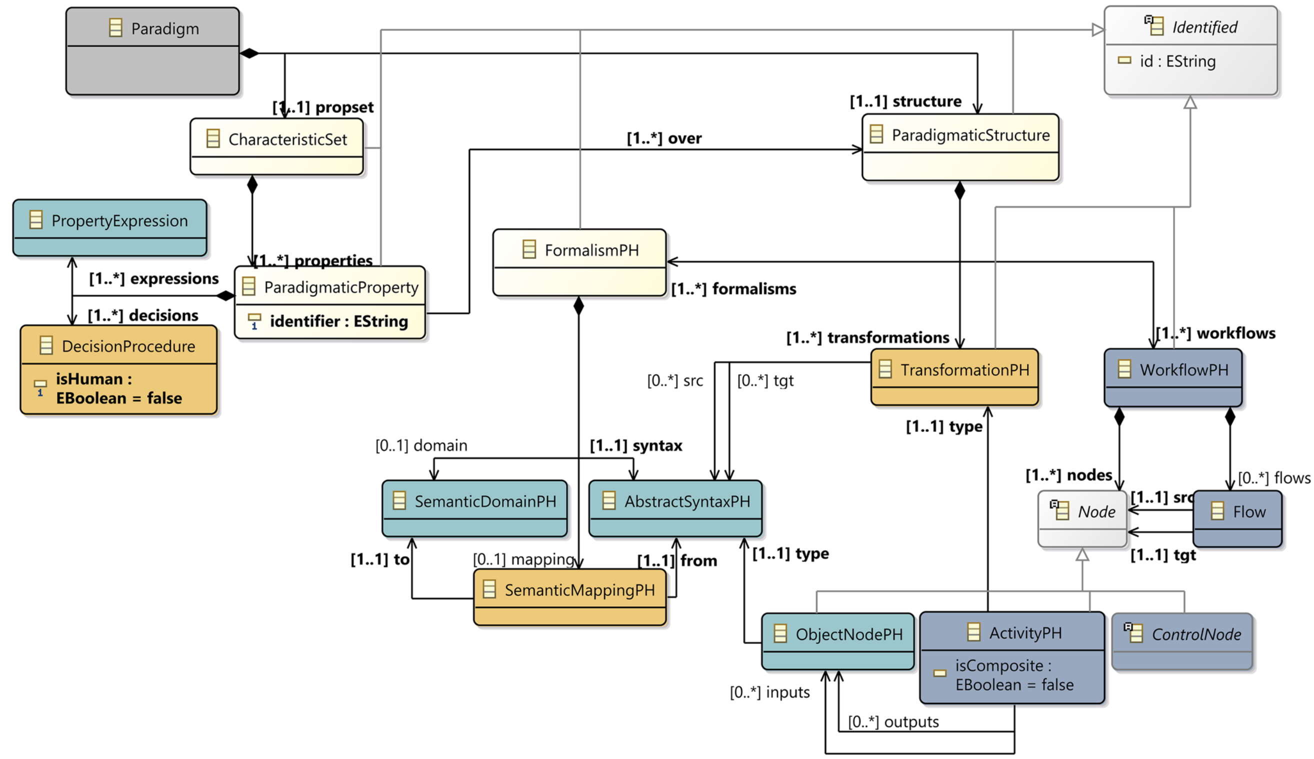


Fig. 3 A metamodel describing the concepts and structure of paradigms. A Paradigm is defined by a set of ParadigmaticPropertys that characterise components consisting of placeholders: FormalismPHs, TransformationPHs and WorkflowPHs

paradigms, namely *properties* over formalisms and workflows. This metamodel, as pictured in Fig. 3, as well as the general principle behind effectively checking whether a given candidate qualifies as, or follows a paradigm, as pictured in Fig. 4, constitutes together our Descriptive Framework for MPM.

From Fig. 3, a paradigm (name) denotes a set of ParadigmaticProperties that capture the essence of the intended paradigm. Many variations or combinations of those properties, grouped in CharacteristicSets, lead to conceptually different paradigms in our framework: for example, Object Orientation with single or multiple inheritance should be named differently. The necessary components of these properties are formally captured by a ParadigmaticStructure, which consists of three interrelated parts: a WorkflowPH capturing the dynamics of how appropriate elements are produced, consumed, and exchanged in an organised fashion within the paradigm, where both activities and objects are typed against TransformationPHs and FormalismPHs, respectively.

We describe in detail each component of the Descriptive Framework, before explaining how to use it concretely to check whether a candidate follows a given paradigm.

3.1 Paradigmatic properties

A ParadigmaticProperty is a property that captures one aspect of the paradigm's essence that is shared by all artefacts that follow it. In other words, such a property is defined "universally" at the level of the paradigm and holds for all artefacts following this paradigm. To check whether it holds or not, a ParadigmaticProperty defines explicitly a DecisionProcedure, which may be automated, or performed by a human (or any combination of both): it may be a mathematical proof, or it may be so difficult to prove that only an agreement among those interested in the Paradigm may be feasible and provide the decision. When all paradigmatic properties are checked to be valid, the artefact then becomes an artefact that qualifies as, or follows, the corresponding paradigm.

3.2 Paradigmatic structure

For a ParadigmaticProperty to be expressed (formally or not), a paradigm needs to define a minimal structure that captures the vocabulary, the concepts and their relationships that the property is about. A ParadigmaticProperty is applied over a ParadigmaticStructure, which is composed of one (or several) workflow(s) with placeholders (WorkflowPH); one (or several) formalism(s) with placeholders (FormalismPH), or one (or several) transformation(s) with placeholders (TransformationPH).

A WorkflowPH links activities with placeholders (ActivityPH) and their object nodes with placeholders (ObjectNodePH) in various ways (sequential or concurrent), described as flows driven by ControlNodes (at this abstraction level, there is no need to distinguish between so-called object and control flows).

A TransformationPH types an ActivityPH by defining a *signature*, i.e. which source(s) and target(s) placeholder formalisms (FormalismPH) the placeholder transformation operates on. We require TransformationPHs to be at least *terminating* (since they are combined in so-called transformation chains [25], they shall always produce outputs), or to *fail* when inputs are not conforming to their source FormalismPH.

A FormalismPH shall at least define, through an AbstractSyntaxPH, the expected structure supporting a ParadigmaticProperty; it may eventually specify a (partial) semantic specification through a SemanticMappingPH that maps elements from the AbstractSyntaxPH to an appropriate SemanticDomainPH. All three of them contain placeholders (as illustrated in Fig. 1 for the inheritance property in OO), allowing arbitrary precision for a ParadigmProperty.

As an example, Fig. 1 describes (part of) the supporting FormalismPH and PropertyExpression for expressing the *inheritance* ParadigmaticProperty, as part of the characteristic set for the Object Orientation paradigm

Note that in this example, we expressed the structure supporting the Inheritance property, and the property itself, in specific formalisms: for the structural part, we selected a MOF-like formalism; for the property, we naturally turned to OCL as it is a standard, and expressive enough for capturing our property of interest. To obtain an explicit specification, many languages of our descriptive framework need to be expressed as valid models of an appropriate formalism. In Fig. 3, we denote by light blue *structural* formalisms (e.g. BNF/Graph Grammars, metamodels, Entity/Relations, or any other suitable ones), and in orange *behavioural* formalisms (GPLs, transformation languages, graph transformations, and so on). Note that both need to be extended to capture *patterns* over candidates (as we suggested and demonstrated using placeholders for the pattern mechanism).

Although the activities comprising a WorkflowPH may be combined freely using ControlNodes and Flows, we require the following conditions to hold, for a WorkflowPH to be well-defined:

– Each ActivityPH is *typed* by a TransformationPH appearing in the same ParadigmaticStructure;
– Each ObjectNode used as input or output of an ActivityPH is *typed* by a FormalismPH, so that
– the type(s) of the ObjectNodes used as input and output of the ActivityPH match the signature of the TransformationPH that types the ActivityPH.

Similar to the structural and behavioural formalisms required for other various components of a ParadigmaticStructure, the elements comprising a WorkflowPH and coloured in dark blue may be part of a (richer) formalism dedicated to the description of workflows (such as UML Activity Diagrams, Business Process Models, etc.); the only constraint is that the Node and Flow concepts are in that formalism. In this paper, we choose Activity Diagrams for this purpose (cf. Sect. 6.4 for a discussion).

As already noticed, our Descriptive Framework admits as valid paradigms definitions that are restricted:

– to only FormalismPH: we assume in this case that there always exists a *default* associated WorkflowPH that allows creating appropriate instances of the formalism it is matched to; or
– to only WorkflowPH: we assume in this case that there exists a *generic, default* FormalismPH that is used by one of the ActivityPH defined inside the ProcessPHs.

This is precisely the case for the examples given in Sect. 2.2, making them valid paradigm definitions in our framework (assuming all ParadigmaticPropertys are effectively specified).

3.3 Checking whether a candidate follows a paradigm

A typical usage for our Descriptive Framework is checking whether a Candidate artefact indeed follows a given paradigm. A candidate is structurally similar to a paradigm's ParadigmaticStructure, with the fundamental difference that components are not merely placeholders anymore. A Candidate may exhibit arbitrarily complex components: the Formalisms may have complicated, intricate syntax and semantics; and the Workflows and associated Transformations (chains) may describe large real-life (industrial, or conceptual) processes related to CPS engineering.

Conceptually, checking that a ParadigmaticProperty holds on a Candidate requires the definition of a Mapping that binds (all) placeholders appearing in the property to the constituents of the Candidate. A mapping may be arbitrarily complex: the languages (metamodels) defining the Candidate may differ radically from the ones used for specifying the ParadigmaticProperty; the semantics of a Candidate may be expressed candidate may be expressed in a different "style" (it is certainly operational for the Candidate in order for it to be executable, while the FormalismPH may use an axiomatic definition to provide constraints over the

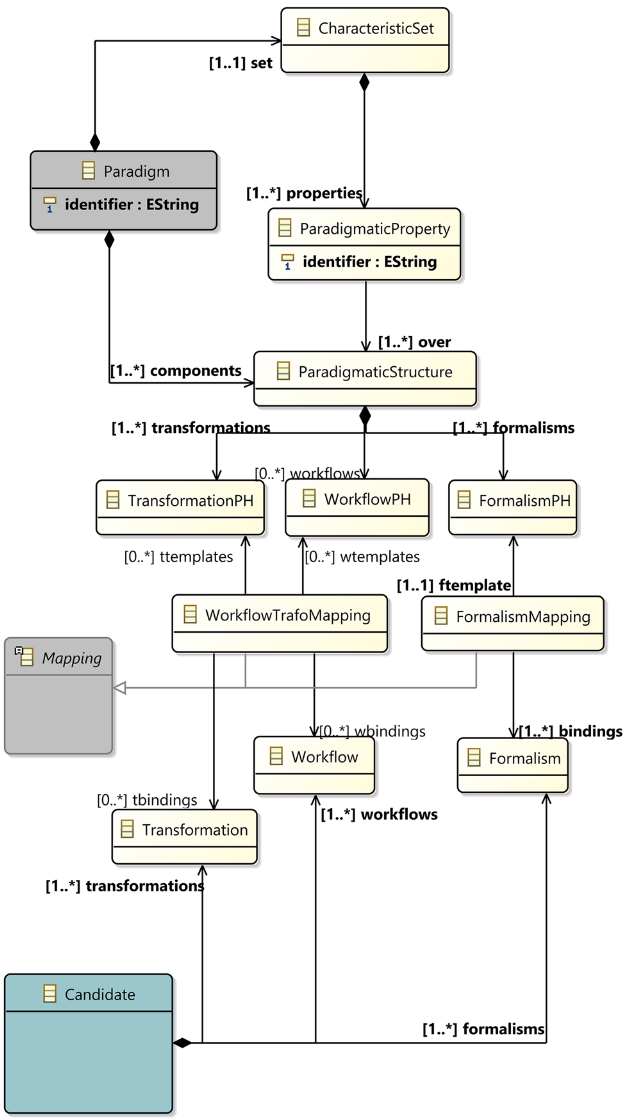


Fig. 4 Checking whether a Candidate follows a given paradigm through a mapping that binds all placeholders in the ParadigmaticStructure's components with concrete elements constituting the Candidate, then applying all DecisionProcedure

semantic domain); and a ParadigmaticProperty may operate at various levels at the same time (syntactic and semantic, just like the inheritance property for OO), making the Mapping sensitive to implementation details. Formally speaking, checking the validity of a ParadigmaticProperty consists of invoking the DecisionProcedure *over* the components the properties apply to (either Transformations, Workflows or Formalisms). but via the Mappings. Note that we define a WorkflowTrafoMapping referencing both the TransformationPH and the WorkflowPH, because candidates may abstract away or refine some parts in the other (i.e. a complex Workflow Placeholder may be realised through a transformation delegated to an external tool, which is then perceived from the Candidate viewpoint as a black box without further control on the internals, thus preventing matching to explicit placeholders).

Formally proving all of the paradigmatic properties required for a candidate to follow a given paradigm may prove extremely tedious, assuming Mappings are actually available. This explains why we expect that the DecisionProcedures associated with a ParadigmaticProperty may well be conducted by humans to overcome this difficult task. Furthermore, as described in the previous section, the formalism choices for expressing the required elements of the Descriptive Framework introduce another burden for performing the proof: as an illustration, if a Candidate for the Object Orientation paradigm captures the Formalism using a different formalism language than the ones we used in Fig. 1, then checking that the Inheritance ParadigmaticProperty holds requires not only a Mapping but additionally an *equivalence* proof between formalisms.

3.4 Final remarks

From our point of view, CPS engineering has largely undervalued the importance of *workflows* in the engineering process. Although manipulating various artefacts (which corresponds to the ActivityPH in our Descriptive Framework, as part of the overall WorkflowPH) is *de facto* a core concern, we believe that explicitly representing *how*, *when*, and to *which purpose* those artefacts interact with each other towards the greater goal of reaching an end product is a crucial part for ensuring deeper understanding of the methodologies and construction processes, but also promotes reuse and adaptation to new constraints. Making workflow pattern descriptions an integral part of our Descriptive Framework is a first step towards recognising this fact and also enables support for the underlying activities with adequate tooling at the level of paradigms (just the way it is for other engineering disciplines, as emphasised, e.g. by Pahl et al. [58] for mechanical engineering).

In our framework, nothing prevents a candidate from being involved in several mappings, allowing it to qualify as various paradigms. As an example, Java, our witness candidate for the *object-oriented* paradigm in Sect. 2.2, may well qualify as an object-oriented, but also as a concurrent GPL, assuming one can provide a proper property characterisation of what concurrency for imperative programming languages may look like. As a consequence, the Mapping component of our Descriptive Framework needs to be separated from the potential candidates; if not for conceptual reasons (as above) then for legacy reasons, because often paradigm elements are built without thinking much of the paradigm they belong, but rather on which kind of issues the element is intended to solve.

When describing informally the kind of formalisms required for capturing the nature of a paradigm, we referred to "*supportive formalisms*" to designate the so-called *meta*-formalisms, i.e. the formalisms in which the listed formalisms (paradigmatic structural, mapping and property, but also the candidate's formalism(s) themselves) are expressed in. In our conceptual metamodel of Fig. 3, we further classified them into two categories: *structural* metaformalisms in blue, which describe structures, and *behavioural* metaformalisms in yellow, which describe computations. We also showed in our tutorial examples from Sect. 2.2 that it is often the case that already existing formalisms may be extended to provide adequate pattern languages for capturing the various components of our descriptive framework (namely ParadigmaticProperty, FormalismPH, TransformationPH and WorkflowPH): we used an extension of UML Class Diagrams and Activity Diagrams to convey the idea of "patterns" that need to be filled by elements of a potential candidate (note that the exact specification and semantics of such extended *placeholder* formalisms remains future work).

We believe that many formalisms may be suitable to be promoted as *pattern/placeholder* formalisms for capturing paradigms' properties when considering suitable research on model typing [17,62,63]. The nature of the relationship between the paradigm's "patterns" and the candidate's matched elements are different from the classical class/instance relationship, since a whole submodel may be matched into a single placeholder. Such "extended" pattern/placeholder languages may be partially obtained through semi-automated processes (e.g. RAMification (Kühne et al [43])), but a precise (semantic) design, specification, and matching process of such languages is left as future work.

The diversity of supporting formalisms gives rise to two crucial, and related, issues:

1. Having different choices for supportive formalisms for the paradigm and a potential candidate requires either that extra effort is put to *translate* one of them (typically, the candidate, which may be defined in various forms) into an appropriate formalism, or to perform mathematical equivalence (or rather, simulation) proofs in order to appropriately match elements. For simplification purposes, we stick to supportive formalisms (UML Class Diagrams and Class Diagrams with placeholders; and Activity Diagrams and Activity Diagrams with placeholders) that correspond to the ones used for potential candidate, to avoid another level of complication; but in practice, this may happen often.
2. Similarly, having different choices impacts the decision procedure, since the paradigmatic properties, as well as the matchings, rely on the paradigm's supportive formalisms. The decision procedure may be seen as a procedure *modulo* the formalisms: here again, equivalence proofs taking into account both the supporting formalisms and the properties are necessary to prove we are manipulating the "same" paradigm.

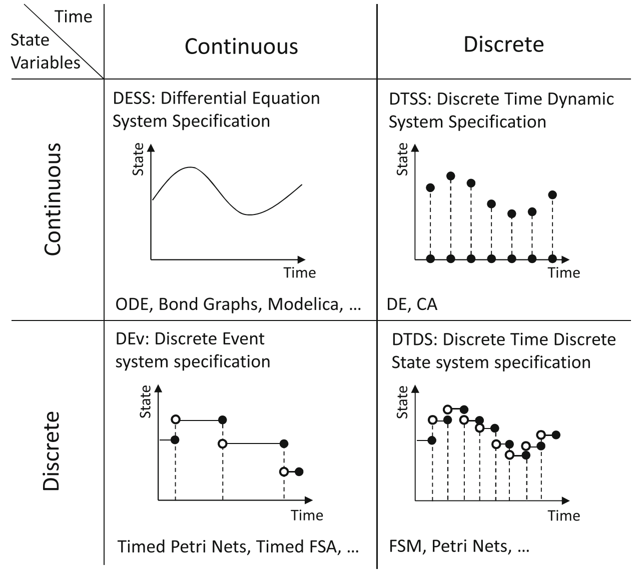


Fig. 5 Classification of modelling abstractions for dynamic systems according to the nature of the *time* and *state* variables [72,79]

4 Two paradigms for CPS: discrete event dynamic systems and synchronous data flow

This section presents two compact examples of paradigms relevant to the engineering of CPSs that have been selected and abstracted to illustrate the concepts of MPM that we strive to convey.

Among the many classifications for CPS modelling abstractions and associated formalisms (cf. Sect. 1 for a quick survey), the simplest and most widespread ones are based on the nature of the representations of the characteristic quantities of a CPS: the *time base* over which the CPS evolves and the *state variables*. Both quantities may be *continuous*, i.e. their domains range over dense domains (such as reals), or *discrete*, i.e. they range over discrete, enumerable domains (such as integers).

Taking a helicopter view, the behaviour of a CPS may be seen as a trajectory that depicts the evolution of state variables over time, which are falling into one of the following categories (cf. Fig. 5 and [79]):

Continuous Variables/Continuous Time leads to complex Differential Equations System Specifications (DESS) where the *constituent* relationships between quantities are captured in the form of differential algebraic equations. Such specifications often require numerical solvers to obtain approximate solutions on digital computers. Typical realisations of this paradigm are Ordinary Differential Equations, Bond Graphs, Equation-Based Object-Oriented Languages such as Modelica, and Analog Electrical Circuit Diagrams.

Continuous Variables/Discrete Time leads to Discrete Time System Specifications (DTSS). These are for example used in sampled system models, representing data periodically obtained from a physical system through sensors. Typical realisations of this paradigm are Difference Equations (DE), and Cellular Automata (CA).

Discrete Variables/Continuous Time leads to Discrete Event dynamic system specifications (DEv). Discrete Event specifications start from the insight that discrete state changes only occur at times of pertinent "events". In between those events, the state does not change and the state trajectory is hence piecewise constant. In a finite time interval, only a finite number of events may occur. Typical realisations of this paradigm are Timed Finite State Machines, Event Graphs and the Discrete Event System Specification (Ziegler's DEVS Formalism [79] which, though Discrete Event, does permit a continuous state space).

Discrete Variables/Discrete Time The other end of the spectrum leads to Discrete Event System Specificatio (DTDS) where discrete state changes only occur at equidistant times. Typical realisations of this paradigm are State Machines.

This section presents the *Discrete Event dynamic systems specification* (abbreviated as *DEv*) and Synchronous Data Flow (abbreviated as SDF) paradigms. We describe both in details within our Descriptive Framework. This choice is guided by three criteria. First, we have selected systems that have opposite natures for the characteristic variables. Second, they are simple enough to convey the necessary concepts for illustrating our Descriptive Framework, while serving as a basis for generalisation to more elaborate CPS models. Third, the combination of those paradigms covers a large spectrum of CPS models used in practice, making them illustrative of the various combinations that exist.

Each paradigm is described systematically using the following approach:

1. We first capture the general requirements from a well-known source that informally describes the paradigm;
2. We translate these requirements within our Descriptive Framework (cf. Fig. 3), using appropriate formalisms;
3. We then present a potential Candidate, specifying its various components (Formalisms, Transformations and Workflows) to a certain extent.
4. We finally apply the checking scenario of Sect. 3.3: we show how Mappings may be (informally) defined, validating that the Candidate indeed follows the paradigm mentioned above.

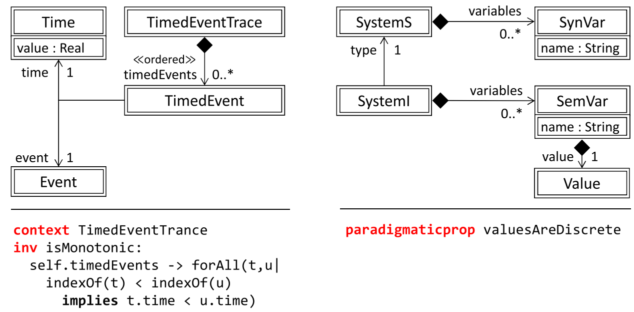


Fig. 6 FormalismPHs and ParadigmaticProperties for the specification of the *DEv* paradigm

4.1 Discrete Event dynamic systems (DEv) paradigm

The *discrete event dynamic system* paradigm uses discrete state variables with continuous time. We illustrate it with the *Timed Finite State Automata* [22].

4.1.1 Paradigm description

From the previous categorisation, we summarise the relevant properties of the *DEv* paradigm and express them in our Descriptive Framework, as depicted in Fig. 6

– The time is continuous: the FormalismPH Time mandates the use of real values for elements matched with Time.
– The system's *dynamics* is captured through timed events: the FormalismPH TimedEventTrace expresses the fact that some elements may be considered as Events that occur at specific time occurrences; the ParadigmaticProperty `isMonotonic` (as expressed in pseudo-OCL) ensures that Events occur at monotonically increasing timestamps.
– The system's (dynamic) state is composed of variables that range over discrete domains: two FormalismPHs describe system specifications (SystemS) and instances (SystemI). A SystemSpecification describes dynamic systems at a high abstraction level, assuming only the declaration of variables (SynVar), while a SystemInstance imposes that variables (SemVar) have values, together with a ParadigmaticProperty that enforces values are actually discrete.

To simplify the description of the *DEv* paradigm, we only consider one fundamental TransformationPH, named Execute, with a trivial WorkflowPH that allows executing the system assuming a given trace.

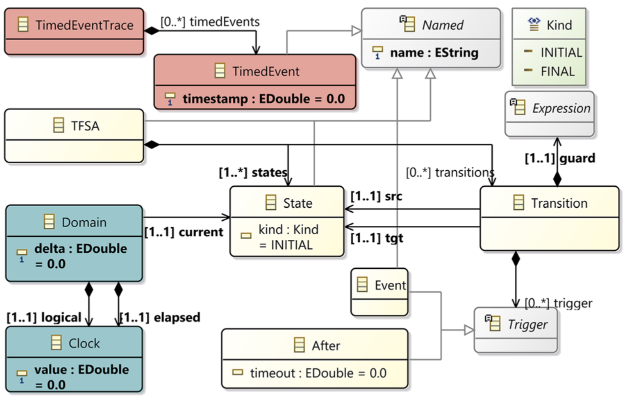


Fig. 7 Metamodels for specifying a TFSA (from Class TFSA); its semantic domain (Class Domain) for accepting a (finite) TimedEventTrace

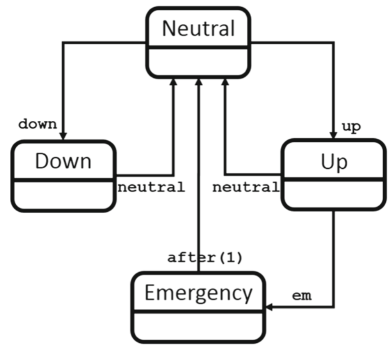


Fig. 8 A simple TFSA conforming to the TFSA domain metamodel of Fig. 7

4.1.2 Candidate: timed finite state automata (TFSA)

When augmented with time constraints, Timed Finite State Automata (TFSA) are powerful formal models, suitable for describing engineered and natural systems in various application domains, which range from sequential circuits, communication protocols, reactive and biological systems. We describe here a simplified *conceptual* formalism for TFSA that may represent concrete implementations in various tools.

Figure 7 describes the TFSA formalism. A TFSA is a Finite State Automaton with an INITIAL and some FINAL states interconnected by Transitions. A TimedEventTrace is a finite list of TimedEvent, consisting of a pair of timestamped event names. A Transition may fire when its Trigger occurs, assuming its guard evaluates to true (the Expression language is left unspecified, as it is not necessary for understanding). When there is an Event Trigger, it should match the current TimedEvent; otherwise, when the Trigger is an After, the Transition fires only when the associated timeout has elapsed, when no other TimedEvent occurs before. The TFSA formalism defines a semantic Domain (also called *configuration*) for specifying an accepting behaviour, provided a specific finite TimedEventTrace: a TFSA accepts a trace iff consuming the TimedEvents composing the trace, in order, results in a FINAL State. The Domain references the current State within the TFSA and manipulates two Clocks: a logical one that records the global time elapse; and a clock used for tracking the elapsed time locally to a State.

Figure 8 shows a simple TFSA that models the behaviour of a (simplified) car Power Window [56] equipped with a three-position command button: when pressed up or down, it indicates the window should move in the appropriate direction; when released, the button produces the neutral event. For safety reasons, when a force is detected resisting the window moving up, the system produces an emergency event, bringing the system into the Emergency mode: after one millisecond, the window stops moving, allowing whatever is obstructing the upward movement to be removed safely.

Listing 1 specifies a procedure execute capturing the behavioural semantics of a TFSA. It operates on a(n instance of a) Domain, assuming a(n instance of a) TFSA and a given (instance of a finite) TimedEventTrace, and proceeds as follows:

Initialise During this phase (Lines 5–7), the various time and state variables are set, pointing the currentState pointing the current State of the computation to the (unique) INITIAL State in the TFSA.

Check Stopping Conditions A loop captures the computation, which runs until no new TimedEvent (Line 9) is present within the given TimedTraceEvent tet, after the currentState is compared to the list of FINAL State of the TFSA.

Perform Step A computation step (Lines 10 – 25) depends on the list of outgoing Transitions of the currentState:

– If an Event Transition labelled with the same name as the current TimeEvent te exists, the Transition is fired (*must*-semantics), changing the currentState to the Transition's tgt;

– Otherwise, if an After Transition is present, it is fired assuming it already reached its timeout (i.e. timeout $\leq$ elapsed). After that, a discrete time step is taken, incrementing both clocks (elapsed and logical) by the predefined delta).

Terminate It remains to check (Line 27) whether the currentState at the end of the computation is a FINAL State.

While explaining the behavioural semantics, we explicitly distinguished separate activities whose dynamics are captured in the Activity Diagram of Fig. 9.

```
procedure execute(d   : Domain,
                  tfsa: TFSA,
                  tet : TimedEventTrace)
do
    d.logical.value = d.elapsed.value = 0
    d.current = tfsa.getInitialState()
    currentState = d.current

    foreach(tevent : tet.timedEvents) do
        outs = tfsa.outgoingTransitions(currentState)
        transition = outs.filter[Event]
            .find[name = tevent.name]
        if(transition != null) then
            currentState = transition.tgt
            d.elapsed.value = 0
        else
            transition = outs.filter[After]
            if(transition != null &&
                transition.timeout <= d.elapsed) then
                currentState = transition.tgt
                d.elapsed.value = 0
            endif
        endif
        d.logical.value += d.delta
        d.elapsed.value += d.delta
    endfor
    return tfsa.getFinalStates().contains(currentState)
endprocedure
```

Listing 1 Algorithmic for the Execute transformation, specifying the behavioural semantics for TFSA.

4.1.3 Mapping

We briefly discuss how to (partially) build the Mapping between the ParadigmaticStructure defining our *DEv* paradigm and the components of our TFSA Candidate, as an instance of the metamodel defined in Fig. 3.

First, the TimedEventTrace metamodel in Fig. 7 maps directly to the TimedEventTrace FormalismPH of Fig. 6: names were kept identical on purpose, since TimedTraceEvents are a rather simple collection structure.

Second, the SystemSpecification may correspond to the TFSA concept, assuming the rest binds appropriately. As state variables for TFSA, which are required by a ParadigmaticProperty to be discrete, we may bind the State concept. As it occurs for TFSA, the class State appears both as a component for the class TFSA, which is matched to SystemS, and as an element in the semantic Domain, which should therefore be bound to SystemI. Since the number of States is always finite (the usual meaning of the "*" in the states reference), it defines a *discrete* domain, thereby validating the ParadigmaticProperty.

Third, the execute procedure presented in Listing 1 maps in a straightforward way to the trivial WorfkflowPH containing the Execute TransformationPH mentioned at the end of Sect. 4.2.2.

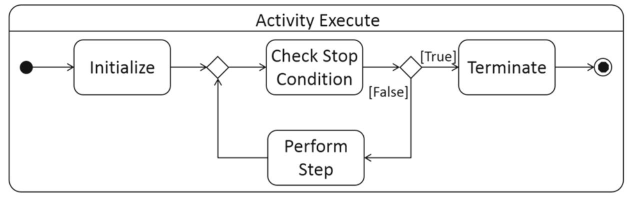


Fig. 9 **Activity Diagram** capturing the dynamics of the activities composing the behavioural semantics common to a TFSA (Listing 1) and a CBD (Listing 2)

4.2 Synchronous Data Flow (SDF) paradigm

The **Synchronous Data Flow** paradigm uses continuous time and state variables, and is illustrated with **Causal Block Diagram** , a formalism representative for many tools such as SIMULINK and SCADE.

4.2.1 Presentation

The Data Flow paradigm [74] describes computations as a special directed graph, with the following features:

Signals represent infinite streams of data, where each data piece is called a *sample*.

Nodes also called *blocks*, represent computation units that *execute* (or *fire*) whenever enough input data become available. Blocks without input can fire at any time. Nodes may be atomic, i.e. performing basic computations (such as adders or multipliers), or composite, thereby encapsulating themselves a subgraph.

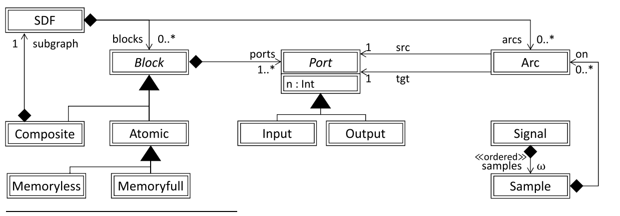
Arcs connect nodes, thus describing how data streams flow throughout the computation blocks.

Executing a Data Flow graph consists of accumulating enough samples within the system, produced by blocks without inputs, and performing the computations within the blocks, thus consuming a number of samples on each input and producing samples on all outputs in a concurrent way. Samples may be reused within the system (for example, in case of cycles) to be used as old samples Messerschmitt [54], but they will not be considered as new once consumed.

The synchronous data flow paradigm [47] is a specialisation of the data flow paradigm where all blocks appearing in a data flow graph are required to be *synchronous*, i.e. each block explicitly defines how many samples are consumed and produced.

4.2.2 Paradigm description

The previous description leads to the following proposal in our Descriptive Framework, as illustrated in Fig. 10:




```
context Arc inv noShortcut:
  self.src.oclIsTypeOf(Input) implies
  not self.tgt.oclIsTypeOf(Output)
```

Fig. 10 FormalismPHs and ParadigmaticProperties for the specification of the *SDF* paradigm (the plain arrow denotes inheritance over placeholder classes)

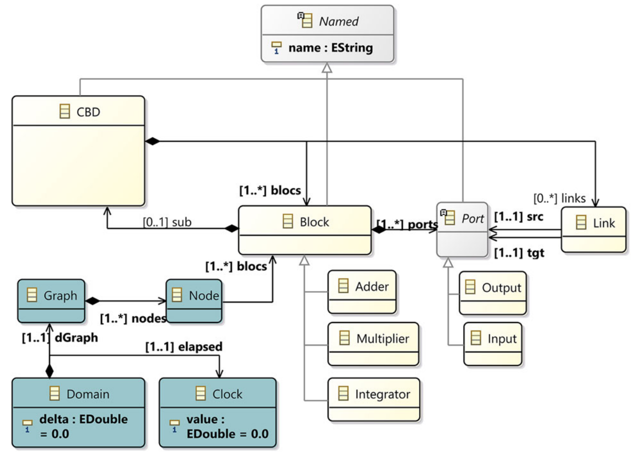


Fig. 11 Metamodels for specifying a CBD (from Class CBD) and its semantic domain (Class Domain) for executing it

– Signals are composed of an infinite, ordered stream of Samples (note the ω multiplicity denoting a collection with an infinite, dynamic number of elements, as suggested by Combemale et al. [14]).
– An SDF has the structure of a *directed* graph with Arcs and Blocks as nodes.
– Blocks possess Ports that explicitly define how many Samples are used (consumed by Inputs, or produced by Outputs).
– Arcs connect Ports, and flow Signals that travel on them instantaneously. Note that a Port may be plugged to several Arcs; only shortcuts are prevented by the noShortcut ParadigmaticProperty, which forbids Arcs to connect as src and tgt Ports of the same Type.
– A memoryfull Block should always define an extra Port corresponding to initial conditions.

To simplify the description of the SDF paradigm, we only consider one fundamental TransformationPH, named Execute, with a trivial WorkflowPH that allows executing the system assuming valid inputs.

4.2.3 Causal block diagrams CBDs

Viewing a CPS as a set of interacting components that may be further decomposed is a natural and intuitive way for breaking its internal complexity. Because they offer an intuitive graphical description in terms of interconnected nodes, Causal Block Diagrams (CBDs) represent a natural formalism for capturing the dynamics of CPSs in a so-called feedback control loop: the evolution of a physical plant is monitored through sensors (thereby introducing a time discretisation), which provide a data stream constantly monitored and analysed by a software that influences back the software plant through actuators. CBDs come in different flavours, depending on the type of blocks that are available for describing a system [20,27]:

– *Algebraic* CBDs only expose mathematical computation blocks (over integers and **boolean** data flows). There is no time progression. They may describe steady-state CPSs occurring once the system has reached a steady state (e.g. an engine after its transition phase);
– *Discrete Time* CBDs extend algebraic CBDs with blocks that introduce *delay*, forcing all algebraic blocks to update their output streams whenever the delay is evaluated. They naturally describe discrete time dynamic systems.
– *Continuous Time* CBDs also extend CBDs, but in a different way: instead of introducing a time step notion with a delay, it extends algebraic CBDs with continuous time, using the mathematical integration and derivative operators. Although theoretically more powerful and more complex than the previous CBD class, they are still suitable for dynamic systems but require numerical discretisation.

CBDs have strong mathematical foundations and largely leverage recent advances in numerical solvers, making their use widespread within several tools (e.g. MathWorks' MATLAB/SimuLink; ANSYS/Esterel SCADE, to only name the most renowned ones). Without loss of generality, and to simplify the presentation, we will also consider the SDF paradigm a *conceptual* formalism for Continuous Time CBD that may be part of concrete tool implementations.

Figure 11 describes the CBD formalism. A CBD is composed of Blocks that possess a number of InputPorts and OutputPorts. Those Ports are Linked appropriately (i.e. a Link connects an output to an input). To simplify the presentation, we only consider three kinds of Blocks: an Adder and a Multiplier (which are both Memoryless) and an Integrator (which is Memoryfull). The semantic Domain for executing a CBD consists of a time step delta, and a dependency Graph (edges are not explicitly represented here) whose Nodes aggregate those Blocks that are cyclically interdependent.

```
1  procedure execute(d    : Domain, cbd : CBD)
2  do
3    d.dGraph =
4        cbd.computeDependencyGraphWithStrongComponents()
5    d.logical.time = 0
6    while(not end_condition) do
7      foreach (scomponent : d.dGraph.nodes) do
8        if(scomponent.size() = 1) then
9          scomponent.nodes.pop().compute()
10       else — Strong Component: compute the whole cycle!
11         scomponent.nodes.compute()
12       endif
13     endfor
14   endwhile
15   d.logical.time += d.delta
16 endprocedure
```

Listing 2 Algorithmic for the Execute transformation, specifying the behavioural semantics for CBD.

Listing 2 describes a procedure execute for capturing the behavioural semantics of a CBD. It operates on a(n instance of a) Domain and a(n instance of a) CBD, and proceeds as follows [27]:

Initialise During this phase (Lines 3–5), the various time and state variables are set: the logical clock is initialised, and the dependency graph with strong components is computed.

Check Stopping Conditions The stopping condition is provided by the user (captured by the end_condition predicate in Line 6) since a CBD computes values at each time step.

Perform Step This step consists of iterating over each Block, in the order of the dependency graph. The (overloaded) Compute procedure depends on the nature of the Block:

- Memoryless A memoryless Block (such as our Adder or Multiplier) simply applies a stepwise basic operation (here, an arithmetic one) on the Samples available on the Input Port, and delivers the result on the Output Port.
- Memoryfull Blocks are split in two categories: a *delay* performs a discrete operation based on previous values of Inputs, thus requiring memory to store such values, while an *accumulator* (like our Integrator) performs an approximation of a continuous behaviour by accumulating the Input (cf. Gomes et al [27] for a detailed explanation; cf. Burden and Faires [9] for details on how numerical approximations may be used for these Blocks).

After having completed the computation of all Block, the logical clock progresses by a delta step value.

The execute procedure may be described as an activity diagram in a similar way as TFSA were, as depicted in Fig. 9. Note that for CBD, the terminate activity is, in fact, empty.

4.2.4 Mapping

Some of the Mappings between the ParadigmaticStructure defining our SDF paradigm and the components of our CBD Candidate are almost straightforward: the CBD metamodel is similar to the FormalismPH for SDF, aside from renaming (e.g. Link trivially binds to Arc), and tagging the proposed Block appropriately (Adder and Multiplier are MemoryLess, while Integrator is MemoryFull). Each Block consumes and produces exactly one Sample on each of its Input and Output Port (assuming the value on the extra Input of MemoryFull Blocks for initial conditions does not change). Note that the timestep in a CBD is implicit, as no syntactic element manipulates it directly. Rather, the timestep corresponds to an evaluation of the full CBD (as shown by the execute procedure, where the time progresses after each full iteration).

Note that the execute procedure described in Listing 2 trivially matches the Execute TransformationPH required in Sect. 4.2.2.

5 Multi-paradigm modelling: combining paradigms

Since CPSs combine physical phenomena with logical decision making, mostly implemented in software, modelling their complex behaviour requires the use of a combination of continuous time models to capture the physical aspects, with discrete time and discrete event models to represent logical computations. Depending on the level of abstraction used, the networking part of CPS may be modelled using either type of models. Furthermore, for many complex CPSs, in order to address the diverse concerns stakeholders may have, complexity is tackled through orthogonal, yet complementary viewpoints. Not only the individual views need to be modelled explicitly, but above all, their often complex interactions and integration.

This section starts by presenting some general mechanisms in engineering that govern the design of a complex CPS. It then proceeds to precisely define one example MPM combinator, namely *embedding*, before applying it to our two CPS-oriented candidates, namely TFSA for the Discrete Event Dynamic System paradigm, and CBD for the synchronous **Synchronous** Data Flow paradigm.

We are aware that embedding is just one of the many combinators applicable to formalisms and workflows, such as extension, unification or self-extension [23], merging [19], and aggregation [36]. However, embedding is popular in practice, and simple enough for us to explain our paradigm combinator concepts concisely. Future work will investigate other paradigm combinators.

5.1 General mechanisms for tackling complexity

Benveniste et al. [5] argue that three basic mechanisms, namely *model abstraction/refinement*, *architectural decomposition* and *view decomposition/merge*, are sufficient to describe any complex CPS engineering effort. In our descriptive framework, these mechanisms may be captured by a combination of TransformationPHs and/or WorkflowPHs, depending on the available machinery, the granularity at which a design needs to be tackled at any point of the CPS engineering life cycle, and the details different engineers need to know about the complete CPS. At this point, it is still not clear whether these mechanisms may themselves be considered as paradigms on their own, or as relationships that paradigms may leverage to capture complex engineering processes (in a similar way to operations over the algebraic structure of paradigm). We simply describe them succinctly, leaving their integration as an extension of our Descriptive Framework.

5.1.1 Model abstraction/refinement

Model abstraction (and its dual, refinement) is used when focusing on a particular set of *properties* of interest. A relationship A between a detailed model m_d and a more abstract model m_a is an *abstraction* with respect to a *set of properties* Π, iff for all properties $\pi \in \Pi$, the satisfaction of π by the more abstract m_a implies the satisfaction of π by the more detailed m_d. This allows one to *substitute* m_d by m_a whenever questions about the properties in Π need to be answered. Substitution is useful as the analysis of properties on the more detailed model is usually more costly than on the abstracted model. Note that the abstraction relationship may hold between models in the same or in different formalisms, as long as for both, the semantics allows for the evaluation of the same properties. When modelling physical systems, continuous domains are frequently used. In that case, a more relaxed notion of substitutability based on *approximation* may be appropriate.

5.1.2 Architectural decomposition/component composition

Architectural decomposition (and its dual, component composition) is used when the problem can be broken into parts, each with an appropriate *interface*. Such an encapsulation reduces a problem to (i) a number of sub-problems, each requiring the satisfaction of its own properties, and each leading to the design of a component and (ii) the design of an appropriate architecture connecting the components in such a way that the composition satisfies the original required properties. Such a breakdown often comes naturally at some levels of abstraction, using appropriate formalisms (which support hierarchy). This may occur when the problem/solution domain exhibits locality or continuity properties. Note that the component models may again be described in different formalisms, as long their interfaces match and the multi-formalism composition has a precise semantics.

5.1.3 View decomposition/merge

View decomposition (and its dual, view merge) is used in the collaboration between multiple stakeholders, each with different concerns. Each viewpoint allows the evaluation of a stakeholder-specific set of properties. When concrete views are merged, the conjunction of all the views' properties must hold. In the software realm, IEEE Standard 1471 defines the relationships between viewpoints and their realisations views. Note that the views may be described in different formalisms.

5.2 Embedding: a simple, powerful MPM combinator

As an orthogonal view to the general mechanisms presented above, there exists the possibility to combine paradigms to form new paradigms through *combinators*, i.e. operators that allow the combination of two artefacts that follow two paradigms (distinct or not). Combinators may even have higher arities, allowing combination of a finite collection of artefacts.

Given the way our Descriptive Framework captures the notion of paradigm, a natural (yet not completely general) way to describe combinators is to proceed in a componentwise fashion:

F-Combinator Combining Formalisms, keeping their default Workflows separate, while ensuring ParadigmaticPropertys that ensure soundness of the operation; or
W-Combinator Combining Workflows, assuming their default Formalisms are distinct, while ensuring soundness.

In this section, we propose to capture a simple binary F-Combinator named *embedding* that we note $\oplus$:

$$\begin{aligned} \oplus : \mathsf{Formalism} \times \mathsf{Formalism} &\to \mathsf{Formalism} \\ (\mathsf{Host}, \mathsf{Guest}) &\mapsto \mathsf{New} \end{aligned}$$

An embedding takes two *source* formalisms (together with their default workflows), the Host and the Guest, each following its own paradigm, and produces a New formalism with two separate, default workflows that may be improved to help co-design the new formalism instances. Note that $\oplus$ is a non-commutative combinator: switching Host, i.e. the formalism that embeds, or is extended with, the Guest, generally results in two radically different results, as we will illustrate in Sects. 5.4 and 5.3.

For the new formalism to be valid, an embedding should:

- Define a new, valid *abstract syntax* based on the abstract syntaxes of the Host and Guest source formalisms;
- Define a new *semantics* that is *conservative*, i.e. if the embedded (syntactic) elements are removed from the new formalism instances, the execution semantics shall *coincide*, as a projection, with each one of the source formalism instance execution semantics.

At a high level, one can see the execution (operational semantics) of an embedding as a three-step process:

1. The host starts the execution, following its semantics;
2. At some specific steps during the execution, corresponding to the embedding, the host delegates the execution to the guest;
3. The guest then proceeds with its own execution semantics;
4. At some predefined steps during the guest's execution, or when something global occurs for the host, the delegation stops and returns to the host.

The specific point where the delegation occurs is defined syntactically, while the mechanisms for delegating from the higher, *macro*-level of the host, to the lower, *micro*-level of the guest and back, is defined in a semantic adaptation (embedding).

For illustrative purpose, we will describe the following embedding, which results in the well-known *hierarchical* TFSA (HTFSA):

$$\text{HTFSA} \triangleq \text{TFSA} \oplus \text{TFSA}$$

5.2.1 Abstract syntax

The pattern described in Fig. 12 (bottom) captures how the resulting paradigm's abstract syntax is constructed: a Director class from the host is extended with a Delegate class from the guest. The Delegate then contains a Delegation where the micro-steps occur. As a guideline for helping identify potential matches, a Director is often a super class extended with particular cases that behave slightly differently from each other.

For building a HTFSA by embedding, we need to match the previous pattern (cf. Fig. 12, top, unnecessary details omitted). We identify as a natural candidate the State class as a Director, which leads to internal computations inside Composite states, performed by an full TFSA as a Delegation.

5.2.2 Execution semantics

The Activity Diagram of Fig. 13 describes a possible recursive operationalisation of the execution semantics in

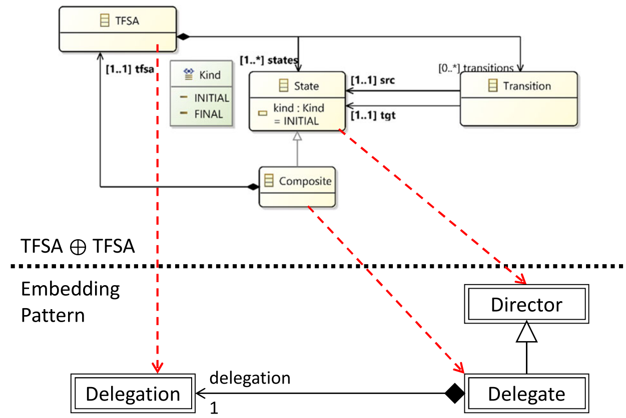


Fig. 12 The Embedding Pattern (bottom) defines how the Abstract Syntax may be built from Host and Guest abstract syntax elements: in the Host, a Director performs macro-steps, and sometimes Delegates computations to the Guest, resulting in micro-steps performed by the Guest's Delegation. In the case of HTFSA, the State class is matched as the Director, using a a full TFSA as a Delegation.

an embedding, by implementing the following algorithm expressed as Activity Diagrams:

1. Starting from the Host, an Initialise phase sets time and system state variables for preparing the computation steps;
2. A CheckStopConditions checks whether this (hierarchical) level's halting conditions are fulfilled. If they are, this level's computation halts: control is transferred back the outer level, eventually performing a Terminate activity for final settings; or the whole computation terminates.
3. If CheckStopConditions are not fulfilled, a PerformStep occurs, making progress for this level's computation;
4. Then, a CheckForDelegation checks whether the current element embeds an internal instance: if this is the case, control is transferred to the inner structure (Delegate::Execute); otherwise, the control loops back to CheckStopConditions for another (macro) step.

The check and eventual call to the Delegate's Execute Transformation (depicted in green) transfers control to the lower level, performing the *micro*-steps embedded inside the current level's *macro*-step (depicted in red). Note that this pattern may occur finitely many times, allowing the embedding of an arbitrary number of levels.

Applying this pattern to the particular case of the HTFSA embedding performs a transfer to the sub-TFSA, while keeping the same Execute specification. Note that this pattern produces a behaviour for HTFSA that is opposite to the one promoted by UML: in case of competition between transitions at different hierarchical levels with identical Events, the *outer*most transition takes priority, following Harel's

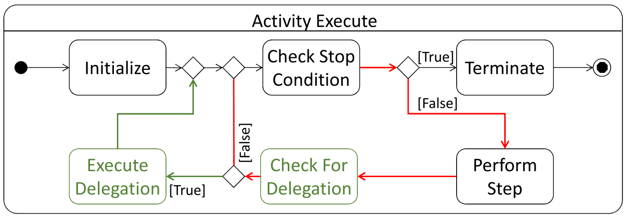


Fig. 13 Pattern expressing the behavioural semantics of an embedding. After a preliminary phase that Initialises necessary variables, a *macro*-step (in red) is performed by the Host. In case of a Delegation at this step (CheckForDelegation), control is transferred to the *micro*-level, after a preliminary phase (InitialiseInternal, corresponding to the Initialise phase, but at the micro-level). When CheckStopConditions fails, it transfers control back to the micro-level, or stops the whole computation if there is none

Statecharts semantics [32] (as opposed to the conventional *inner*most choice in UML).

5.3 Embedding CBD into TFSA

Many CPSs evolve through so-called *running modes* [51], i.e. their behaviour changes significantly depending on high-level, clearly identifiable *modes*. For example, regulatory systems in biology identify potential deviations from a normal course of action (such as cell mitosis, DNA replication, metabolic regulation and so on), and take measures to recover, thus exhibiting two clear modes; robot arms in a factory exhibit different behaviour depending on the way they move in space in order to avoid hurting the humans working around them, or to hit an obstacle, thus making clear distinctions when operating in either secure or risky environments; autonomous electric vehicles introduce several driving modes for handling snow, allowing user-controlled drifting for circuit driving, or avoiding obstacles dangerous for the occupants, thus exhibiting clear distinctions on how to manage power, drive trains and so on depending on potential dangers or road conditions.

Consider as a small example of such a CPS, a bouncing ball that may be kicked from time to time [73]: a ball starts free-falling from a predefined height; it will eventually collide with the ground, then bounces up again with reduced energy; sometimes it is kicked, adding a predefined velocity. To model such a system, we immediately notice three modes: a FreeFall mode describes the ball's free fall, following Newton's laws; the (artificial, infinitesimally short) Collision mode describes the moment the ball hits the ground and bounces up, going again in free fall; and the Kick mode represent a kick, adding to the ball's upward velocity. At a high level of abstraction, this small system switches from one of those modes to one of the others, depending on clearly defined events, where each mode describes the system's dynamics with continuous, physical (Newtonian) laws. There are two paradigms at play in this scenario:

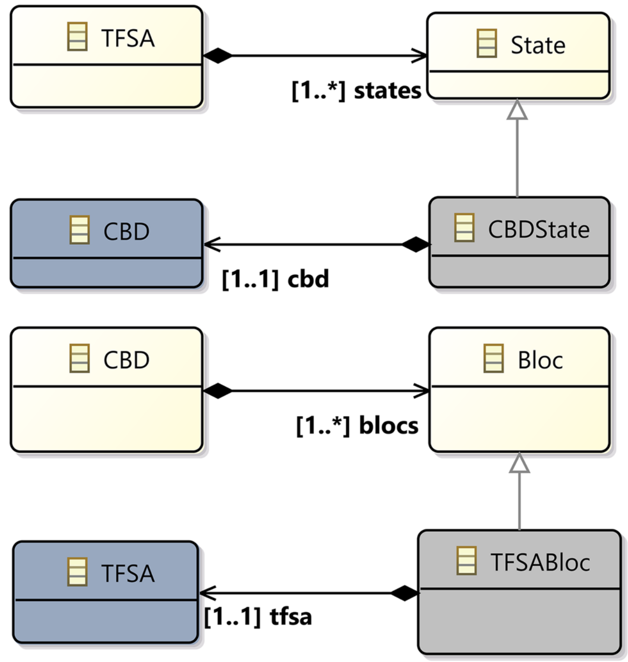


Fig. 14 Concretising the Embedding Pattern of Fig. 12 (bottom) for TFSA ⊕ CBD (top) and CBD ⊕ TFSA (bottom) (Delegate in grey and Delegation in red)

– at an outer level, describing modes where switching occurs when particular events are identified corresponds to the Discrete Event Dynamic System paradigm;
– at an inner level, in each mode, representing the dynamics of a Newtonian physical system may be approximated in a Synchronous Data Flow paradigm.

The presence of an outer and an inner level suggests to embed an SDF formalism into a DEv formalism, following the procedure described previously:

Abstract Syntax Modes may be captured by States; therefore, matching the State class as a Delegate seems appropriate. The Delegation is composed of a full CBD for capturing the various physical laws governing the free falls (up and down) and the kick-up (cf. Fig. 14).

Execution Semantics Two instances of the Execute Activity Diagram of Fig. 9 may be composed following the pattern described in Sect. 5.2.2: the macro-step would follow the activities described for the behavioural semantics of TFSA (Listing 1), while the micro-step would embed the activities for the behavioural semantics of CBD (Listing 2). Note that to effectively allow a simulation of the whole system, a new time step delta should be computed as the maximum common divisor of the TFSA semantic Domain's delta and the CBD semantic Domain's delta.

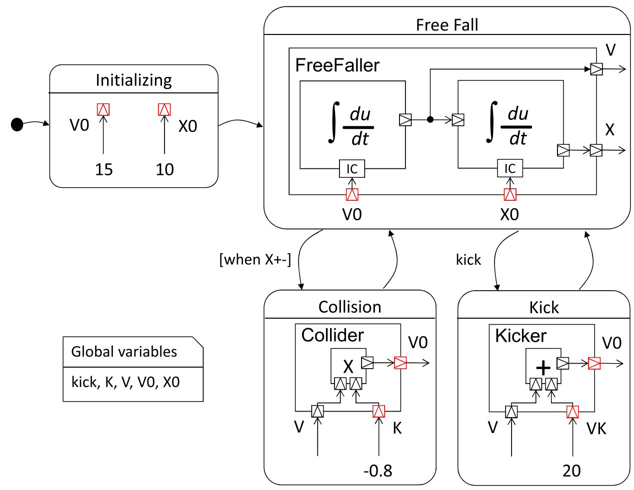


Fig. 15 Model of the Kickable Bouncing Ball: after Initialising the necessary state variables, the ball is in FreeFall, following Netwton's Free Fall Law, then Colliding, thus bouncing. Sometimes, the ball gets Kicked, allowing it to momentarily gain upward speed. The Global Variables are shared by the CBD inside the States

The ⊕ combinator only provides guidelines for embedding: some syntactic and semantic adjustments need to be provided to obtain a full fledged formalism. In this case, two elements need to be taken care of to enable communication between both formalisms:

– Since CBDs continuously compute outputs from input when activated inside a State, they need persistent GlobalVariables to enable communication between instances in various State.
– Possibly new Triggers may need to be defined to capture the so-called *level/zero-crossing* phenomenon, i.e. producing inside the environment an Event when some continuous variables exceed a predefined threshold [80].

As a result, Fig. 15 depicts a possible instance of the embedding TFSA ⊕ CBD that captures the behaviour of the kickable bouncing ball. The GlobalVariables are declared outside the TFSA, and two specific Events (namely when +- and when -+) detect the moments when the ball reaches the lowest (on the ground) and highest positions during falls.

5.4 Embedding TFSA into CBD

Many CPSs are, from an abstract viewpoint, so-called feedback control systems ([4]), i.e. they are composed of two (or more) subsystems that are connected so that each influences the other(s), with the particularity that at least one of these subsystems (often realised as a software component) senses the operations of the other subsystems through various sensors, compares the sensed behaviour to a desired behaviour, and computes corrective actions that are applied through actuators. Such interconnected, strongly coupled CPSs are notoriously difficult to analyse, making modelling and simulation a crucial enabler in the large-scale development of such systems.

Consider again the small CPS example of a car's Power Window, introduced earlier in Sect. 4.1.2, but now taking physical effects into consideration. A driver has at his disposal two buttons Up and Down, which manually command a motor that moves a driver-side window. For safety reasons, the Window is also equipped with a sensor that detects a resistive Force against the upward movement, helping detect whether an object obstructs the Window's course. One possible way to check the safety of the system is to simulate it and to check that a reasonable Force always leads to halting the window's upward motion. A possible (simplified) model would compute the position of the Window, given the multiple inputs (provided by the user's manual commands and the sensor) and some predefined parameters (corresponding to the Friction the window's frame imposes on the Window during its movement, and the motor's linear force Motor). We can distinguish two different paradigms that are involved in a Control/Command pair:

– at an outer level, the Window's movement simply follows Newton's Second Law, since the overall mass of the system (frame + motor + window) stays constant.
– at an inner level, deciding which direction the Window should move in may be modelled in a discrete way by analysing the window's state over time and detecting the emergency cases due to excessive resistive force.

From an abstract viewpoint, the Window's movement may be simulated using the SDF paradigm (using a discretisation of its equations of motion), while the control part may be described through the *DEv* paradigm, suggesting to embed a *Dev* formalism into an SDF one, following the procedure presented above:

Abstract Syntax In a CBD, the Block class plays the role of the Director, attaching as a Delegation a full TFSA (cf. Fig. 14).

Execution Semantics A construction similar to the previous case may be used, this time using CBD as the macro-step and TFSA as a micro-step.

As a result, Fig. 16 depicts a possible instance of the embedding CBD ⊕ TFSA, for modelling (part of) the behaviour of the Power Window CPS.

6 Related work

Our work proposes an explicit definition of the notion of modelling paradigm, which is a generalisation of the notion of programming paradigm to the more general domain of

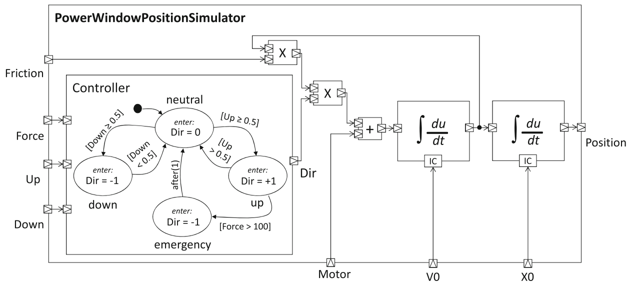


Fig. 16 Partial model of a power window in a car. The first CBD Block continuously computes in which direction the Window (motor) moves, transmitting the information to the second Block, which effectively realises the movement

modelling. Over the years, a plethora of programming languages have been developed to deal with the heterogeneity of software systems. The notion of programming paradigm [31,78] was proposed more than 30 years ago to categorise the different approaches or styles used by the many different programming languages. This lead to the rich research field of multi-paradigm programming. We did, however, not find any work making the notion of programming paradigm as explicit and precise as we propose in this work. Rather, the notion of programming paradigm is expressed in natural language and varies slightly from one author to another. Van Roy [68] proposed a more precise definition where a programming paradigm is defined as "[...] a set of programming concepts, organised into a simple core language called the paradigm's kernel language". Even this definition is neither precise, nor does it propose, or even identify the need for a procedure to decide whether a programming language is based on a given paradigm.

We find the same issue with MPM, which as mentioned earlier, originated from the Modelling and Simulation Community in 1996. While the initial work of the COST Action IC1404 MPM4CPS[2] proposed an ontology for the domain of MPM for CPS, we do not find a precise definition of the notion of a modelling paradigm in the ontology. There is, however, a body of work well suited to support multi-paradigm modelling, such as the composition of modelling languages, the composition of analyses, the composition of tools and the composition of workflows. Furthermore, while research has produced a variety of interesting textbooks on modelling for CPS, such as Alur [2], Lee and Seshia [47], Taha et al [65], these usually employ selected modelling techniques and do not cover the multi-paradigm aspects of CPSs.

The related work regarding each of these topics is discussed in the following subsections.

2 http://mpm4cps.eu.

6.1 Composition of Modelling Languages

The composition of modelling languages is closely related to multi-paradigm modelling as composed languages often comprise different formalisms (e.g. UML class diagrams for the Object-Oriented description of structures, State Machines that describe state-based behaviour, and OCL to describe constraints of the overall system). To this end, software language engineering [36] produced a variety of formalisms, such as

- the integrated syntax definitions of MontiCore [35], Neverlang [66], and Xtext [6];
- methods to define well-formedness rules, including OCL [33] or the Name-Binding Language NaBL [71] of Spoofax;
- model transformation techniques and frameworks, such as ATL [40], T-Core [64], or the Epsilon Transformation Language ETL [41].

For such language definition formalisms, the composition techniques range from embedding and merging of abstract syntax definitions [19,35], over matching grammar non-terminals by name [66] and importing syntactic elements from other DSLs [6], to the integration of interpreters or code generators [10,45]. All of these have in common that their compositionality is limited to the level of their formalisms, i.e. yet there is no software language reuse technology that considers composing the intended usage workflows (e.g. compiling, transforming, validating) that come with them.

Language workbenches [24] span technological spaces by providing and combining multiple formalisms, such as grammars and template languages for code generation [66] or reference architectures for metamodels [34] and interpreters for model execution [76] to support engineering multiple aspects of modelling languages. Such workbenches come with powerful tools and documented workflows describing how to engineer languages with the given formalisms. The workflows are usually given in natural language, which severely hampers reasoning about the compatibility with other workflows. Also, often the mappings between their supporting formalisms (e.g. metamodelling techniques and code generators) are not modelled explicitly but encoded in the tooling. A formal basis for MPM can enable the making explicit of workflows and their relations to formalisms, thus facilitating language composition not only across formalisms, but also across workbenches.

6.2 Composition of analyses

Another field of research closely related to MPM is the composition of analyses, since composed analyses often comprise different formalisms (e.g. discrete event systems for reasoning about event-based communication, queuing networks for resource utilisation analysis and logical programming for constraint checking).

One established way to realise analysis composition is simulator coupling and co-simulation. Distributed Interactive Simulation (DIS) [38] is a decentralised approach to simulator coupling, where the state of the analysis is shared between all participants of the simulation. The successor of DIS is High-Level Architecture (HLA) [37] standard. Coupling information is stored by a central manager which enables the combination of analyses. An overview of the state of the art of co-simulation is presented by Gomes et al. [26].

All of these approaches have in common that their compositionality is limited to the level of their formalisms and to information exchange between partial analyses implemented in tools. There is, however, no modularisation and composition concept for analyses on a semantic level. A formal basis for MPM can serve as a foundation for modularisation and composition of analyses on a semantic level.

6.3 Composition of software tools

Combining different formalisms usually implies combining the tools that operate on models in these formalisms. Tools are commonly integrated to form so-called toolchains. However, the field lacks methodical or theoretical foundations for systematically combining such tools across various domains.

Co-Simulation [26], as already mentioned in the previous section, is one specific area where tools composition is supported by foundational work. Co-simulation allows one to combine existing simulation tools into a integrated simulator, with some guarantees of correctness. The Functional Mockup Interface (FMI)[3] standard provides Functional Mock-Up Units (FMU) that can be combined/orchestrated using standardised interfaces.

The Open Services for Lifecycle Collaboration (OSLC) Initiative[4] proposes a set of specifications that enable the integration of any kind of software development tools. It builds on the W3C RDF (Resource Description Framework) to describe resources shared by tools, linked data to relate these resources and a REST (REpresentation State Tansfer) interface to expos the tool APIs as Web services for their integration, as techniques to enable the preview, creation and selection of links between resources. OSLC strongly relies on Web technologies which may limit performance. It also lacks technology agnostic foundations.

The SPIRIT framework [39] for model and data integration and toolchain development tries to provide a more all-encompassing foundation. One advantage of this approach is that it considers the evaluation of how well the developed toolchains perform and adopts a service-oriented approach. For evaluation, metrics are defined for the capabilities of individual tools within a toolchain, and the interoperability of the whole toolchain. SPIRIT integrates several open standards such as the GOPPRR (Graph Object Property Point Role Relationship) metametamodel, the Web Ontology Language (OWL), the FMI and Business Process Modelling Notation (BPMN) for workflow modelling. However, it is not clear whether the approach requires that existing formalisms are re-implemented based on this metametamodel.

6.4 Composition of workflows

While the MPM community recognised that the explicit specification of MBSE workflows (as, for example, described in this paper) is needed, the workflow management community has long understood the usefulness of explicitly modelling service composition and choreography (e.g. [18,67]) using appropriate formalisms.

Service Composition and Business Process Composition [21,44] are two well-known approaches. Service Composition is usually split into two broad categories: *static* composition, which includes orchestration, i.e. one service orchestrating the others, and choreography, i.e. each service describes its interactions, for which different formalisms and languages have been developed over the years such as WS-BPEL, WS-CDL and OWL-S; and *dynamic* composition, which uses semantic annotations as proposed by Lautenbacher and Bauer [44].

Many Business Process Composition algorithms have been proposed based on graphical notations: for example, Brockmans et al. [7] proposed to model business processes through Petri Nets, which are annotated with domain ontologies using similarity computation and aggregation. However, none of these approaches from the workflow management community considers the composition of multiple formalisms.

7 Discussion

Our Descriptive Framework for MPM is the first approach to enable the systematic integration, use, and evaluation of the variety of paradigms necessary to successfully engineer CPSs. Built on the generic concepts of formalisms, workflows, model operations, and their integration, the framework is agnostic to the kind of systems it is applied to. While we consider this beneficial for the applicability of our theory, specific instances of the use of MPM, with predefined formalisms and workflows for specific challenges, can be useful in more limited contexts.

Our Framework shows that specific metaformalisms for describing formalisms, transformations, and workflows are

[3] https://fmi-standard.org/.

[4] https://open-services.net/.

necessary to achieve enough precision to be able to explicitly check whether a paradigm candidate follows a paradigm. This choice of metaformalisms imposes a particular view on MPM. Other choices such as functional or logical views might yield different results. However, as metamodels have been successfully employed to describe (parts of) the world in software engineering, we consider this choice well-suited to describe the foundations of MPM. Nonetheless, freedom in this choice entails that when paradigm candidates are described using formalisms different from those used in this paper to capture the paradigmatic structure, mechanisms are required to (dis)prove their equivalence and compatibility. This will complicate establishing relations between these paradigms and demands further research. The existing research on the topic of semantic equivalence is seen as a possible starting point.

This freedom of choice also extends to the property languages of choice (such as the metamodel patterns used in this paper). When the formalisms to specify paradigms are fixed and integrated, suitable and more specific property languages can be derived automatically using modelling language engineering techniques (such as ProMoBox [55], among other approaches). When this choice is not fixed, the paradigms used for property description and property checking need to be integrated properly as well. When no automated methods exist to check the equivalence of properties expressed in different formalisms, a manual proof might be required.

The *Physical* part in CPS introduces the need for computationally *a*causal models in order to capture the constitutive physical laws of such systems, which may well be expressed through an *acausal paradigm*. Note how Equation-based Object-Oriented Languages such as Modelica supporting the acausal paradigm still only capture mathematical relationships. Still, they may not capture all constraints imposed by the laws of physics. That requires even more physics-oriented paradigms, those based on Power Flows [29] as used in Bond Graphs [8]. On the other hand, combining inherently causal "*cyber*" components and aspects of CPSs, also implies the combination of causal paradigms (i.e. refinements such as the Data Flow or the State Automata paradigms that we illustrated in this paper) with acausal paradigms. This combination does fit in our proposal for a Descriptive Framework and is indeed the heart and soul of CPSs. However, for pedagogical reasons and for the purpose of illustration when presenting this Framework, we have restricted the illustrative formalisms and workflows to the simplest possible, yet keeping the key ingredients to illustrate how combinations of such paradigms may look like. Further application of our Descriptive Framework to more elaborated acausal paradigms and their possible combinations is left as future work.

Our framework is also completely agnostic with respect to the specific way the integration of two (or more) paradigms is done, as this integration highly depends on the constituent paradigms, as well as on the purpose of the integration. We illustrated paradigm integration with an example (namely TFSA $\oplus$ CBD for mode automata) where one paradigm describes the system's structure, while the other captures the state-based behaviour of the system's elements. Moving towards, for example, assembly lines would require the integration of geometry (supported by Computer-Aided Design) with kinematics and rule-based assembly knowledge, opening the way to radically different types of integration. Our extensional perspective for joining the paradigms' specifications is the foundation for integration in our MPM theory. This does require further restrictions to be identified, e.g. information about the formalisms, workflows, and the intentions of integration (as it has been identified for Model Transformations [49]).

The combinations of paradigms discussed in the examples focus on the formalisms and detail corresponding compositions. As sketched in Fig. 2, the combination of workflows demands for composition operations such as activity embedding (or similar combinations) that, again, depend on the formalisms of choice. Note also that in practice, many operations that should be enforced at the formalism level may be delegated to the workflow part as an external operation. For example, checking the validity of a CPS design may require the knowledge of other views or components of the overall system, thereby relying on legacy procedures to ensure consistency, which will naturally take the form of an activity. In future work, we will detail this for various workflow formalisms and their usage in concrete situations.

Our vision of applying MPM includes structuring the engineering of CPSs by making the paradigms of the different stakeholders explicit and machine-processable, and, ultimately, applying our theory to foster automation in Systems Engineering. This may include building, deriving, and validating tool ensembles for engineering specific CPSs as well as making the cooperation between the different stakeholders through the paradigms explicit. Moreover, we expect this vision to enable predicting various qualities of the engineering process as well as of the CPS product.

To properly integrate different paradigms and prevent operating on incompatible paradigms, we must be able to identify formalisms and workflows belonging to a certain well-defined paradigm. To this end, *decision procedures* need to be established to determine whether formalisms and workflows belong to a certain paradigm, that can subsequently be integrated. Of course, these procedures are also highly dependent on the paradigms in question and may not be automatically decidable in all cases.

Paradigms may be related to one another, e.g. through extension, refinement, or substitutability. These relationships may form the basis for reuse of paradigm-based analyses, proofs, tools, etc. We illustrated a rather simplistic example for Object Orientation (with single vs. multiple inheritance).

This is subject to ongoing work and might relate to the notion of model types [17,30] for the structure of formalisms and to the notion of semantic refinement [60] for the behaviour specified in workflows.

To capitalise on the foundations of MPM, the construction, analysis, and integration of paradigms should, ultimately, be supported through automation. Therefore, software tools are needed that capture workflows related to paradigms, such as analysing whether a set of paradigms can be integrated to achieve certain results, to store, query, and retrieve paradigms from repositories, and more. The functional requirements for such tools and repositories demand further research and form the core of MPM engineering as a discipline.

The examples presented throughout the paper are carefully selected to clarify the concepts of MPM that we strive to convey. Consequently, these are compact and cannot cover the complete landscape of paradigms and their combinations necessary to engineer a sophisticated CPS. In the future, we will investigate selecting and combining specific paradigms to design, engineer, and deploy CPSs to present the application of our framework in the large.

MPM advocates using the most appropriate formalisms. This may lead to different components and views expressed in different formalisms with different semantics. The burden is on the modeller to prove equivalence—if that is needed or indeed even possible. However, once formalisms and workflows have been explicitly modelled, implementing a decision procedure becomes possible. This will most likely require a community to stick to a particular "style" of modelling. If multiple styles are needed, proofs of equivalence may not be possible. Then again, a community may agree on equivalence until the converse is proven.

8 Conclusion

This paper proposed a structural Descriptive Framework for Multi-Paradigm Modelling. A paradigm P is defined as a set of characteristics, so-called *paradigmatic properties*, that requires a *paradigmatic structure* to be expressed explicitly. This paradigmatic structure captures "universal" concepts expressed through placeholders and shared by all artefacts qualifying as, or following P. The placeholders are intended to be mapped to the concrete constructs defining potential candidates. This enables decision procedures associated with the paradigmatic properties to be performed to validate whether a paradigm candidate follows P. To tackle the heterogeneity and complexity of CPSs, it is often necessary to combine multiple paradigms to adequately capture all facets of a CPS. This calls for Multi-Paradigm Modelling. To that end, we have explored a first paradigm combinator, namely *embedding*, and have shown how to systematically build a valid paradigm candidate for the resulting multi-paradigm combination.

The Descriptive Framework presented in this paper is a first step towards more formal foundations for MPM for CPSs, which future research can build upon. For instance, during the COST Action IC1404, we actively collected and classified several industrial paradigmatic scenarios involving various workflows and formalisms. From this work, an interesting library of CPS paradigms currently used in industry may follow. Such a library will allow researchers and practitioners to reflect and build upon. It will also provide a further validation of the structures described in our Descriptive Framework. Capturing other paradigm combination operators observed in practice would also contribute to the exploration of the various ways MPM is already used in industry for modelling and simulating complex CPSs. Based on the understanding gained in this work, of different paradigms and their interaction for modelling and analysing complex CPSs, we will explore a feature-based decomposition and composition of modelling languages and analyses. Ultimately, a better understanding of the different paradigms that are in place to model CPSs and of their integration can yield better modelling, analysis, design, and optimisation tools. This will contribute to more efficient engineering practices of future CPSs.

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References

1. Abadi, M., Cardelli, L.: A Theory of Objects. Springer, New York (1998)

2. Alur, R.: Principles of Cyber-Physical Systems. MIT Press, Cambridge (2015)
3. Amrani, M., Blouin, D., Heinrich, R., Rensink, A., Vangheluwe, H., Wortmann, A.: Towards a formal specification of multi-paradigm modelling. In: International Conference on Model Driven Engineering Languages and Systems Companion, pp. 419–424 (2019)
4. Åström, K.J., Murray, R.M.: Feedback Systems: An Introduction for Scientists and Engineers. Princeton University Press, Princeton (2012)
5. Benveniste, A., Caillaud, B., Nickovic, D., Passerone, R., Raclet, J.B., Reinkemeier, P., Sangiovanni-Vincentelli, A., Damm, W., Henzinger, T.A., Larsen, K.G.: Contracts for system design. Foundations and trends in electronic design automation. **12**(2–3) (2018). https://www.amazon.co.uk/Contracts-System-Foundations-Electronic-Automation/dp/1680834029
6. Bettini, L.: Implementing Domain-Specific Languages with Xtext and Xtend. Packt Publishing Ltd, Birmingham (2016)
7. Brockmans, S., Ehrig, M., Koschmider, A., Oberweis, A., Studer, R.: Semantic alignment of business processes. In: Proceedings of the Eighth International Conference on Enterprise Information Systems: Databases and Information Systems Integration, pp. 191–196 (2006)
8. Broenink, J.F.: Bond graphs: A unifying framework for modelling of physical systems. In: Foundations of Multi-Paradigm Modelling for Cyber-Physical Systems, pp. 15–44. Springer (2020)
9. Burden, R.L., Faires, J.D.: Numerical Analysis. Cengage Learning (2015)
10. Butting, A., Eikermann, R., Kautz, O., Rumpe, B., Wortmann, A.: Modeling language variability with reusable language components. In: International Conference on Systems and Software Product Line (SPLC'18). ACM (2018)
11. Cambridge University Press: Cambridge Dictionary (2020). https://dictionary.cambridge.org/dictionary/english/paradigm. Accessed 25 Mar 2020
12. Carreira, P., Amaral, V., Vangheluwe, H.: Foundations of Multi-Paradigm Modelling for Cyber-Physical Systems. Springer, New York (2020)
13. Clavel, M., Durán, F., Eker, S., Lincoln, P., Martí-Oliet, N., Meseguer, J., Talcott, C.: All About Maude. How to Specify, Program and Verify Systems in Rewriting Logic. Springer, A High-Performance Logical Framework (2007)
14. Combemale, B., Thirioux, X., Baudry, B.: Formally defining and iterating infinite models. In: International Conference on Model Driven Engineering Languages and Systems, pp. 119–133 (2012)
15. Cooper, D.: Standard Pascal User Reference Manual. W. W. Norton, New York (1983)
16. Corradini, A., Dotti, F.L., Foss, L., Ribeiro, L.: Translating java code to graph transformation systems. In: International Conference on Graph Transformation, pp. 383–398 (2004)
17. De Lara, J., Guerra, E.: A posteriori typing for model-driven engineering: concepts, analysis, and applications. ACM Trans. Softw. Eng. Methodol. **25**(4), 1–31 (2017)
18. Decker, G., Weske, M.: Interaction-centric modeling of process choreographies. Inf. Syst. **36**(2), 292–312 (2011). https://doi.org/10.1016/j.is.2010.06.005
19. Degueule, T., Combemale, B., Blouin, A., Barais, O., Jézéquel, J.M.: Melange: A meta-language for modular and reusable development of DSLs. Proceedings of the 2015 ACM SIGPLAN International Conference on Software Language Engineering, pp. 25–36 (2015b)
20. Denckla, B., Mosterman, P.J.: Formalizing causal block diagrams for modeling a class of hybrid dynamic systems. In: Proceedings of the 44th IEEE Conference on Decision and Control, pp. 4193–4198, (2005). https://doi.org/10.1109/CDC.2005.1582820
21. Dumas, M., Rosa, M.L., Mendling, J., Reijers, H.A.: Fundamentals of Business Process Management, 2nd edn. Springer, New York (2018)
22. El-Fakih, K., Gromov, M., Shabaldina, N.V., Yevtushenko, N.: Distinguishing experiments for timed nondeterministic finite state machines. Acta Cybern. **21**(2), 205–222 (2013)
23. Erdweg, S., Giarrusso, P.G., Rendel, T.: Language composition untangled. In: Proceedings of the Twelfth Workshop on Language Descriptions, Tools, and Applications, pp. 1–8 (2012)
24. Erdweg, S., Van Der Storm, T., Völter, M., Tratt, L., Bosman, R., Cook, W.R., Gerritsen, A., Hulshout, A., Kelly, S., Loh, A., et al.: Evaluating and comparing language workbenches: existing results and benchmarks for the future. Comput. Lang. Syst. Struct. **44**, 24–47 (2015)
25. Fritzsche, M., Gilani, W., Lämmel, R., Jouault, F.: Model transformation chains in model-driven performance engineering: experiences and future research needs. In: Modellierung, pp. 213–220 (2011)
26. Gomes, C., et al.: Co-simulation: a survey. ACM Comput. Surv. **51**(3), 49 (2018)
27. Gomes, C., Denil, J., Vangheluwe, H.: Causal-block diagrams: a family of languages for causal modelling of cyber-physical systems. In: Carreira, P., Amaral, V., Vangheluwe, H. (eds.) Foundations of Multi-Paradigm Modelling for Cyber-Physical Systems, pp. 97–125. Springer, Cham (2020). https://doi.org/10.1007/978-3-030-43946-0_4
28. Gosling, J., Joy, B., Steele, G.L., Bracha, G., Buckley, A.: The Java Language Specification. Java SE, 8th edn. Addison-Wesley Professional, Redwood City (2014)
29. Grainger, J.J., Stevenson, W.D., Chang, G.W.: Power Systems Analysis. Mc Graw Hill, New York (2015)
30. Guy, C., Combemale, B., Derrien, S., Steel, J.R., Jézéquel, J.M.: On model subtyping. In: European Conference on Modelling Foundations and Applications, pp. 400–415. Springer (2012)
31. Hailpern, B.: Guest editor's introduction multiparadigm languages and environments. IEEE Softw. **3**(01), 6–9 (1986). https://doi.org/10.1109/MS.1986.232426
32. Harel, D., Naamad, A.: The STATEMATE Semantics of Statecharts. ACM Trans. Softw. Eng. Methodol. **5**, 293–333 (1996)
33. Heidenreich, F., Johannes, J., Karol, S., Seifert, M., Thiele, M., Wende, C., Wilke, C.: Integrating OCL and textual modelling languages. In: International Conference on Model Driven Engineering Languages and Systems, pp 349–363. Springer (2010)
34. Heinrich, R., Strittmatter, M., Reussner, R.H.: A layered reference architecture for metamodels to tailor quality modeling and analysis. IEEE Trans. Softw. Eng. (2019). https://doi.org/10.1109/TSE.2019.2903797
35. Hölldobler, K., Rumpe, B.: MontiCore 5 Language Workbench Edition 2017. Aachener Informatik-Berichte, Software Engineering, Band, vol. 32. Shaker Verlag (2017)
36. Hölldobler, K., Rumpe, B., Wortmann, A.: software language engineering in the large: towards composing and deriving languages. Comput. Lang. Syst. Struct. **54**, 386–405 (2018)
37. IEEE Ieee standard for modeling and simulation (m amp;s) high level architecture (hla)—framework and rules. IEEE Std 1516-2010 (Revision of IEEE Std 1516-2000) pp 1–38 (2010). https://doi.org/10.1109/IEEESTD.2010.5553440
38. IEEE: IEEE Standard for distributed interactive simulation—communication services and profiles. IEEE Std **12782–1995**, 1–20 (1996). https://doi.org/10.1109/IEEESTD.1996.80824
39. Jinzhi, L.: A framework for cyber-physical system tool-chain development: A service-oriented and model-based systems engineering approach. PhD thesis, KTH Royal Institute of Technology (2019)
40. Jouault, F., Allilaire, F., Bézivin, J., Kurtev, I., Valduriez, P.: ATL: a QVT-like transformation language. In: Companion to the 21st

ACM SIGPLAN symposium on Object-oriented programming systems, languages, and applications, pp. 719–720. ACM (2006)
41. Kolovos, D.S., Paige, R.F., Polack, F.A.: The epsilon transformation language. In: International Conference on Theory and Practice of Model Transformations, pp. 46–60. Springer (2008)
42. Kuhn, T.: The Structure of Scientific Revolutions. Chicago Press, Chicago (2012)
43. Kühne, T., Mezei, G., Syriani, E., Vangheluwe, H., Wimmer, M.: Explicit transformation modeling. In: MODELS Workshops, pp. 240–255 (2009)
44. Lautenbacher, F., Bauer, B.: A survey on workflow annotation and composition approaches. In: Proceedings of the Workshop on Semantic Business Process and Product Lifecycle Management (2007)
45. Leduc, M., Degueule, T., Combemale, B.: Modular Language Composition for the Masses. In: Proceedings of the 11th ACM SIGPLAN International Conference on Software Language Engineering, pp 47–59. ACM (2018)
46. Lee, E.A., Messerschmitt, D.G.: Static scheduling of synchronous data flow programs for digital signal processing. IEEE Trans. Comput. **36**(1), 24–35 (1987)
47. Lee, E.A., Seshia, S.A.: Introduction to Embedded Systems: A Cyber-Physical Systems Approach. MIT Press, Cambridge (2016)
48. Liu, S.H.: Design Space Exploration for Distributed Real-Time: A Software Product Line Engineering Approach for Design and Analysis of Component-Based Distributed Real-Time and Embedded Systems. VDM Verlag (2010)
49. Lúcio, L., Amrani, M., Dingel, J., Lambers, L., Salay, R., Selim, G., Syriani, E., Wimmer, M.: Model transformation intents and their properties. SoSyM **15**(3), 647–684 (2014)
50. Manifesto, A.: Manifesto for agile software development. (2001) See https://agilemanifesto.org/. Accessed 2 Aug 2020
51. Maraninchi, F., Rémond, Y.: Mode Automata. A New Domain-Specific Construct For The Development of Safe Critical Systems. Science of Computer Programming (2003)
52. Merkow, M.: Secure, Resilient, and Agile Software Development. Auerbach Publications, New York (2019)
53. Merriam-Webster : Merriam-Webster Online Dictionary. (2020). https://www.merriam-webster.com/dictionary/paradigm. Accessed: 25 Mar 2020
54. Messerschmitt, D.G.: A tool for structured functional simulation. IEEE J. Sel. Areas Commun. **2**(1), 137–147 (1984)
55. Meyers, B., Vangheluwe, H., Denil, J., Salay, R.: A framework for temporal verification support in domain-specific modelling. IEEE Trans. Softw. Eng. (TSE) **93**(12), 1045–1061 (2017)
56. Mosterman, P.J., Sztipanovits, J., Engell, S.: Computer-automated multiparadigm modeling in control systems technology. IEEE Trans. Control Syst. Technol. **12**(2), 223–234 (2012)
57. Oxford University Press (2020) Oxford English Dictionary. https://www.oed.com/view/Entry/137329. Accessed: 25 Mar 2020
58. Pahl, G., Beitz, W., Feldhusen, J., Grote, K.H.: Engineering Design. A Systematic Approach. Springer, New York (2007)
59. Przybyłek, A., Morales-Trujillo, M.E. (eds.): Advances in Agile and User-Centred Software Engineering. Lecture Notes in Business Information Processing, vol. 376. Springer, New York (2019)
60. Rumpe, B., Wortmann, A.: Abstraction and refinement in hierarchically decomposable and underspecified CPS-architectures. In: Lohstroh, M., Derler, P., Sirjani, M. (eds.) Principles of Modeling: Essays Dedicated to Edward A. Lee on the Occasion of His 60th Birthday, LNCS 10760, pp. 383–406. Springer, New York (2018)
61. Stärk, R.F., Schmid, J., Börger, E.: Java and the Java Virtual Machine: Definition. Verification Validation. Springer, New York (2014)
62. Steel, J., Jézéquel, J.M.: On Model Typing. Software And Systems Modeling (2007)
63. Sun, W., Combemale, B., Derrien, S., France, R.B.: Using Model Types to Support Contract-Aware Model Substitutability. In: European Conference on Modelling Foundations and Applications, pp. 118–133 (2013)
64. Syriani, E., Vangheluwe, H., LaShomb, B.: T-core: a framework for custom-built model transformation engines. Softw. Syst. Model. **14**(3), 1215–1243 (2015)
65. Taha, W., Taha, A.E.M., Thunberg, J.: Cyber-Physical Systems: A Model-Based Approach. Springer, New York (2020)
66. Vacchi, E., Cazzola, W.: Neverlang: a framework for feature-oriented language development. Comput. Lang. Syst. Struct. **43**, 1–40 (2015)
67. van der Aalst, W.M.P., Mooij, A.J., Stahl, C., Wolf, K.: Service Interaction: Patterns, Formalization, and Analysis, pp. 42–88. Springer, Berlin (2009). https://doi.org/10.1007/978-3-642-01918-0_2
68. Van Roy, P.: Concepts, Techniques, and Models of Computer Programming, Chap Programming Paradigms for Dummies: What Every Programmer Should Know, pp. 9–47. MIT Press, Cambridge (2012)
69. Vangheluwe, H., Vansteenkiste, G., Kerckhoffs, E.: Simulation for the Future: Progress of the ESPRIT Basic Research working group 8467. In: European Simulation Symposium (ESS), SCS (1996)
70. Vangheluwe, H., Vansteenkiste, G.: A multi-paradigm modeling and simulation methodology: Formalisms and languages. In: European Simulation Symposium (ESS), SCS, pp. 168–172 (1996)
71. Wachsmuth, G.H., Konat, G.D.P., Visser, E.: language design with the Spoofax language Workbench. IEEE Softw. **31**(5), 35–43 (2014)
72. Wainer, G.A.: Discrete-Event Modeling and Simulation: A Practitioner's Approach. CRC Press, Boca Raton (2009)
73. Wainer, G.A., Mosterman, P.J. (eds.): Discrete-Event Modeling and Simulation: Theory and Applications. CRC Press, Boca Raton (2010)
74. Watson, I., Gürd, J.G.: A practical data flow computer. IEEE Comput. **15**, 51–57 (1982)
75. Wegner, P.: Dimensions of object-based language design. SIGPLAN Not. **22**(12), 168–182 (1987)
76. Wende, C.: Language Family Engineering—with Features and Role-Based Composition. PhD thesis, Technische Universitaet Dresden (2012)
77. Wimmer, M., Kramler, G.: Bridging Grammarware and Modelware. In: Workshop in Software Model Engineering, pp. 159–168 (2005)
78. Zave, P.: A compositional approach to multiparadigm programming. IEEE Softw. **6**(05), 15–18 (1989). https://doi.org/10.1109/52.795096
79. Zeigler, B.P., Muzy, A., Kofman, E.: Theory of Modeling and Simulation: Discrete Event and Iterative System Computational Foundations. Academic Press, London (2018)
80. Zhang, F., Yeddanapudi, M., Mosterman, P.J.: Zero-crossing location and detection algorithms for hybrid system simulation. Int. Fed. Autom. Control **41**(2), 7967–7972 (2008)

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Multi-paradigm Modelling for Policy-driven Socio-technical Systems

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Abstract
Today's socio-technical systems, intertwined with fast-changing cyber-physical infrastructures, are becoming increasingly complex and must be able to cope with major unexpected events - e.g. health, economic and ecology crisis; digital innovation, pandemics, etc. As a result, these systems, which are governed by policies, experience rapid developments in their regulation requirements. In this context, traditional policy-making processes are slow relative to the present pace of changes they face, often leading to outdated inappropriate governance. We present a research plan for developing a highly configurable framework and set of tools to help policy making by providing support to better specify, analyse, monitor and assess socio-technical systems, taking into account governing policies and their impacts. The framework is inspired from model-based systems engineering approaches, which have been successful for Cyber-Physical Systems, to better formulate, characterise and analyse socio-technical systems and their governing policies. It makes use at its heart of Multi-Paradigm Modelling, to develop, reuse and integrate appropriate domain-specific modelling languages and tools, views and analyses to better address policy making of nowadays rapidly changing complex heterogeneous socio-technical systems.

Keywords
Socio-Technical Systems, Cyber-Physical Systems, Self-Adaptive Systems, Multi-Paradigm Modelling, Model-Based Systems Engineering, Model Analyses, Simulation

1. Introduction

Modern societies, increasingly intertwined with fast-changing cyber-physical infrastructures (i.e. hence leading to socio-technical systems), experience rapid developments in their regulation requirements. In this context, traditional policy-making processes are rather slow relative to the present pace of societal changes, often leading to outdated policies – i.e. 'institutional lag'. Evolving such regulations involves several processes, including: collecting sufficient relevant information, assessing the latest changes, determining unsuitable or lacking policies, proposing suitable updates and going through various debating, negotiation and approval processes, before implementing actual amendments or extensions.

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As Socio-Technical Systems (STSs) are becoming increasingly complex, so are the policy-making processes that aim to regulate them. This, in turn, leads to situations where policy-makers are overloaded and unable to keep-up with latest developments. Notable difficulties stem from the lack of resources to sustain long-term policies, the preference towards short-term planning within the electoral process, and, more essential with respect to this work, the lack of standardised frameworks and tools for monitoring and assessing policy impacts [1].

Modern Cyber-Physical Systems (CPSs) experience similar challenges, chiefly related to the complexity of their adaptation management processes in a context of rapid and unpredictable changes. Research solutions have been developed to deal with such challenges – spanning from initial data collection, system modelling and analysis (e.g. data-mediation frameworks [2], digital twins [3], Multi-Paradigm Modelling (MPM) [4]) and all the way to runtime decisions and system adaptations (e.g. self-aware [5] and self-managing systems [6], decentralised and multi-scale controllers [7], models at runtime [8], self-integrating systems [9]).

In this vision paper, based on our expertise with some of the above-mentioned topics, and on our experience on policy-making for STSs of the forestry management domain [10, 11, 12], we survey existing systems engineering and self-adaptation solutions for complex CPSs that can potentially be adapted to better develop policies for modern STSs. Our objective is not to propose a new policy making process, but rather to allow improving existing ones using multi-paradigm modelling to support their specification and application, inspired from successful solutions issued from systems engineering and self-adaptive goal-oriented, multi-scale control CPSs, which exhibit characteristics similar to STSs. As a survey of approaches, we do not present any specific case studies but focus on similarities between the domains of STSs CPSs to establish an initial research plan. Developing specific case studies will be part of future work.

We start by introducing minimal notions on STSs and existing approaches for policy making in section 2. We then introduce CPSs and associated successful engineering methods in section 3, including the main approaches on which our framework will build (i.e. Goal-Oriented Requirements Engineering (GORE), Design-Space Exploration (DSE) and Goal-Oriented Multi-Scale Control Systems (GOMSS). In section 4, we introduce enablers for theses approaches (i.e. Model-Based Engineering (MBE) and its Multi-Paradigm Modelling (MPM) extension). We then present the blueprint of our approach based on these preliminary notions in section 5 – this includes the existing modelling languages and tools it may reuse, as well as the languages and tools that we aim to develop for policy making activities and domain-specif modelling in the planned case studies. We conclude the paper in section 7.

2. Policy Making for Socio-Technical Systems

STSs involve wide-spread interactions amongst people and technologies, hence integrating complex social and technical infrastructures with human behaviour. The term STS and its theory was coined during World War II to characterise systems such as coal mines in England [13]. The purpose of STS theory was to study how these systems' management processes could be improved so as to increase overall system performance and quality in people's work lives.

STSs management involves governance, which relies on a set of policies developed by policy-makers. Policy-making is a complex process that involves many stakeholders, often pursuing different or incompatible interests. It may also span over long periods during which stakeholder interests may vary. As policies are strongly context-depend, they should consider, e.g., national, economic, political, cultural and social structures.

For instance, [14] presents an interesting overview of the conceptual and methodological aspects of policy-making for the European Training Foundation (ETF). It introduces basic notions related to policy-making and its different approaches developed over time. We will briefly present some of these notions so that we can later-on emphasise on their similarities with systems engineering methods to illustrate how our proposed framework can build upon these to better support policy making with adequate modelling languages and tools.

Policy-making processes build upon a set of policy analysis activities, which mainly investigate alternative policy options by gathering and integrating the advantages and inconveniences of each option. It is a problem-solving activity that attempts to predict the consequences of alternative courses of action. Numerous perspectives and frameworks exist for policy analysis. The ETF outlines three main approaches – namely, the *analycentric*, the *policy process* and the *meta-policy* – each dealing with problems at three different scales. The *analycentric* approach typically focuses on individual, technical problems at the micro-scale and aims to identify the most effective and efficient solution in technical and economic terms (e.g. the most efficient resource allocation). The *policy process* approach usually focuses on political problems (e.g. involved stakeholders) at the meso-scale, aiming to determine employed processes and means and to explain the stakeholders' role and influences. Problem solutions are identified by changing the relative power and influence of certain groups (e.g., enhancing public participation and consultation). Finally, the *meta-policy* approach focuses on the structural problems of the system and its context, at the macro-scale (e.g. an economic system or political institution). It aims to explain the contextual factors of the policy process– i.e., what are the political, economic and socio-cultural factors influencing it.

Such policy analyses constitute the backbone activities of overall policy-making processes, aiming to specify and validate, at least to a minimal level, the fact that a set of policies fits the problem that must be solved within a targeted STS. Within this overall process, the ETF proposes: first, to use elements of the policy process and meta-policy approaches to set policy priorities; and secondly, to employ the analycentric approach when formulating the actual policy option.

Other policy-making support solutions are also discussed in [14], such as the policy cycle framework and the policy network perspective. The *policy cycle* aims to split complex policy-making processes into manageable steps, breaking them down into sequential stages, examining what happens within each individual stage, and assuming that each stage influences the following one. The *policy network* offers a different way to tackle policy-making complexities. It concentrates on the (meta-)policy process and the relations amongst the actors (i.e. the network) who participate in it, seeking to explain policy outcomes in relation to these characteristics.

The policy-making process proposed by the ETF combines the aforementioned policy cycle with the policy networks. Here, policy networks are approached as a model of collective decision making– an exchange process between actors operating within a market to gain control and influence over resources. This leads to the overall-policy making process depicted in Fig. 1. Fig. 2 shows the detailed steps decomposing the Policy Formulation stage of Fig. 1.

One key aspect as stressed by the ETF is that there is no single or best way to conduct policy

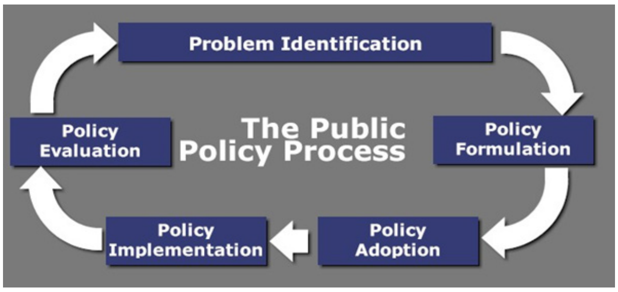

Figure 1: The public policy process proposed by the ETF [14].

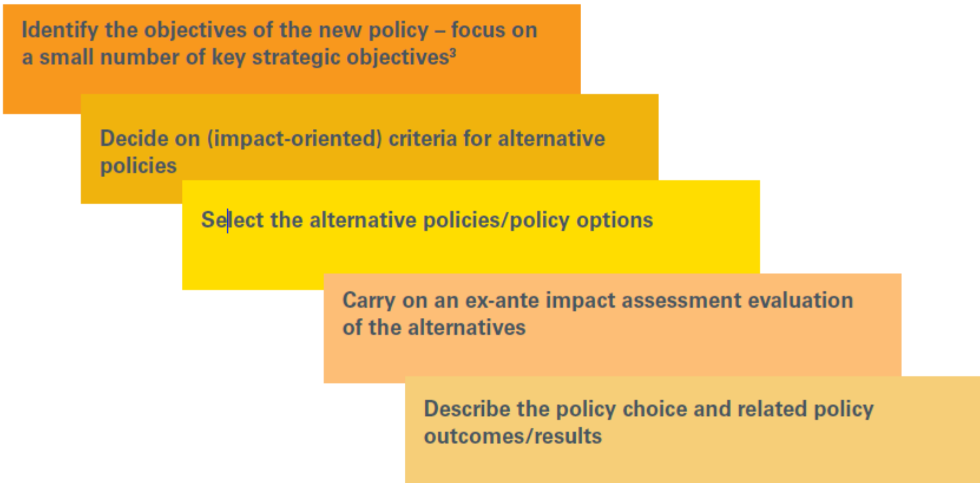

Figure 2: Detailed steps for the *Policy Formulation* stage of Fig. 1 [14].

analyses, due to the multi-faceted nature of policy analyses. Such is also the case for systems engineering where each organisation will typically need to customise standard development processes in order to satisfy organisation and project specific needs. Hence, a policy making framework must allow to seamlessly customise processes and tools by allowing to define and integrate new activities and workflows as needed by the specific policy-making organisations, projects and STSs under consideration.

Another interesting aspect mentioned by the ETF regarding policy analysis is the importance of problem identification, as many policy-making failures are due to solving the wrong problem (rather than to proposing wrong solutions to the right problem). This means that significant effort should go into the formulation of the policy problem. This difficulty is also largely observed in systems engineering, for which several requirements engineering approaches have been developed, which as we will see later could be beneficial when applied to policy making.

Finally, the ETF note that under these circumstances, there is an increasing need to professionalise policy making and its activities to ensure effective governance of these processes and the capacity to anticipate problems. This will help avoiding traps such as policy overload, which happens when governments develop policy plans that are too complex or too vague, containing too many priorities. This results in focus less fragmented priorities leading to endless stream of ad-hoc initiatives. This was illustrated repeatedly during the COVID19 crisis, e.g., in France. The lesson here is that policy plans must be actionable and clear, so as to ensure wide-spread adoption by concerned stakeholders. Therefore, better tool support to policy making is required to help avoid falling into these traps.

3. Engineering Cyber-Physical Systems

Compared to STSs, Cyber-Physical Systems (CPSs) are also complex systems, yet generally excluding the more unpredictable human dimension. The CPS term emerged around 2006 at the National Science Foundation in the United States [15] to identify systems that integrate multi-physical processes (e.g. mechanical, electrical, biochemical) and computational processes (e.g. control, signal-processing, logical inference, planning); and that typically run within uncertain environments. These systems are part of many of our daily activities and drive innovation in important domains (e.g. Automotive, Avionics, Civil Engineering, Industry 4.0, Robotics, smart systems).

While CPS are generally engineered to be predictable – especially for safety-critical systems, e.g. air planes – including humans in the loop brings about new dimensions of complexity and unpredictability. Indeed, the latest trends in CPS development research is to better include human factors – considering a system's human actors and their socioeconomic context [16]. This brings about the new challenge of dealing with highly unpredictable entities. Therefore, CPSs indirectly inherit several characteristics of STSs.

Similar to complex STSs, for which policy-making processes have been developed, well-known engineering processes have been proposed for different kinds of engineered systems; and for CPSs in particular. The most well-known is the Systems Engineering process promoted by the INCOSE (International Council on Systems Engineering) [1].

Systems Engineering is a trans-disciplinary integrative approach covering the entire system life-cycle– starting from its development, its operation, maintenance and all the way to its disposal. It consists of establishing stakeholders' goals and required system functionalities, including an appropriate system life-cycle model, process approach and governance structures; while taking into account the system's complexity, uncertainty, change and variety.

A critical activity in the systems engineering process – often called Design Space Exploration (DSE) – is to consider alternative system designs and configurations, so as to find the best design for the given requirements. Based on these results, system synthesis, verification and validation from the system design can be performed. Fig. 3 illustrates the overall systems engineering process. We can easily map several of its stages to the ones of the policy making process of Fig. 1. For instance, each process starts with a stage including strong emphasis on problem identification, as explicitly stated for policy making. This also takes place for system engineering during the customer needs analysis stage. The Policy Formulation stage on the policy making side, which consists of formulating adequate policies to solve the identified

[1] INCOSE: https://www.incose.org/

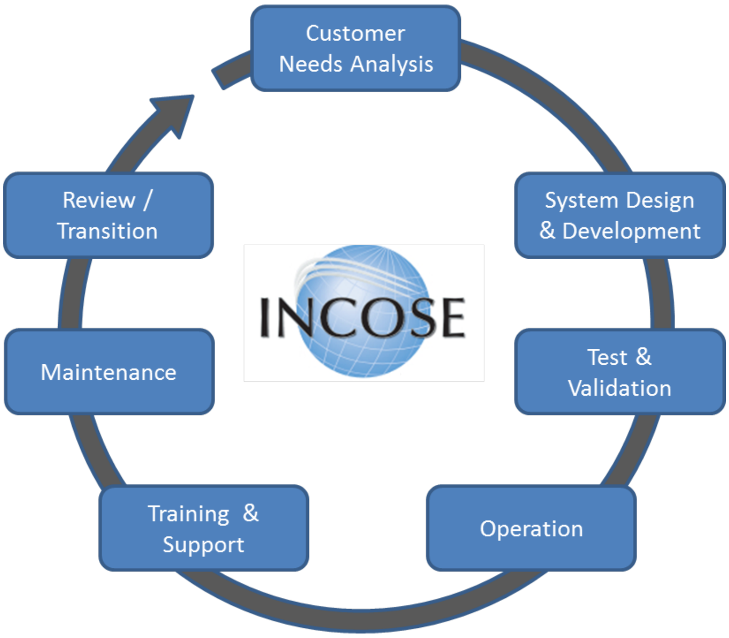

Figure 3: The systems engineering process as proposed by the INCOSE.

problem, corresponds to System Design and Development on the systems engineering side, where engineers Specify a solution to the identified customer problem. We note, from Fig. 2, that each of these solution building stages include alternative solutions evaluation steps in order to come up with the best solution to the specified problems. Policy Adoption and Implementation stages correspond to the systems engineering Tests & Validation and Operation stages, and the Policy Evaluation stage to the Review / Transition stage of systems engineering. Finally, we note that each process circularly comes back to its initial problem identification stage with the whole process being applied iteratively for both policy making and systems engineering cases.

3.1. Goal Oriented Requirements Engineering (GORE)

As we have seen previously, similar to policy-making, systems engineering also emphasises the problem and solution domains. The problem phase has been given high attention by the Requirements Engineering (RE) community. The notions of goals, or requirements, were developed to specify the problem with the solution expressed via system architecture. However, it is difficult to set a precise boundary between the problem and solution parts. Developing a solution is iterative, and design choices often implying new more detailed requirements to be added to the problem part, and so on.

Nevertheless, experience showed that most problems are introduced during the RE stage. This triggered the development of Goal Oriented Requirements Engineering (GORE) approaches [17, 18, 19, 20]. For instance, the KAOS approach defines four complementary and interrelated views on the system and its environment:

- *Goals* representing owners, users, business managers, regulations, etc., which are analysed taking into account conflicts and their resolution.
- *Responsible agents*, both human and machine from the system and its environment, which captures system structure in terms of subsystems and their interactions.
- The specific *problem domain* represented by concepts and their relationships.
- *Agent behaviours* that agents must exhibit in order to achieve goals as well as possible.

The combination of these different views on the system allowed developing several activities to better analyse and validate requirements and significantly improve system design and development.

3.2. Goal-Oriented Multi-Scale Control Systems (GOMSS)

While GORE traditionally focuses on the system's offline specification and development, the high unpredictability of execution environments requires to push these processes into the run-time (i.e. during system execution). This is the case for most complex STSs, e.g. smart homes and cities, power grids, autonomous vehicle networks, robotic swarms and integrated Industry 4.0 systems-of-systems.

To deal with runtime changes, while requiring minimal human intervention and ideally no service disruption, such systems must adapt themselves to dynamic changes in their internal resources, execution environment and even targeted goals. Several relatively recent research areas have been tackling this challenge, notably including Autonomic Computing (AC) [6], Organic Computing (OC) [21], Self-Adaptive Systems (SAS) and Self-aware Computing (SeAC) [5].

To enable self-adaptation, systems generally feature internal control feedback loops – for system and context *monitoring*; problem detection and *analysis*; solution *planning*; and *execution*. Such feedback loops rely on various types of *knowledge* (e.g. system, environment and goal models), which can be updated and extended at runtime (e.g. learning).

In addition to specifying the design and algorithms of such control feedbacks (i.e. defining *how* the system should self-adapt), more recent solutions have also considered explicitly specifying the goals of such control feedbacks (i.e. *what* the self-adaptive system should achieve). Hence, goal-oriented self-adaptive systems go beyond the dynamic selection of predefined adaptive behaviours, allowing the system to learn and discover new adaptation behaviours, as suited for dealing with problematic situations that couldn't be predicted at design-time. E.g. [22] propose to enable systems to self-integrate from an extensible set of control components, which can be discovered at runtime, so as to achieve explicitly-specified goals when new problems occur.

Considering the very nature of most complex systems (i.e. typically composed of a large number of interconnected entities), the *scalability* of self-adaptation solutions is always a major issue. Various forms of hierarchical approaches have been proposed to handle this issue, either via generic architectures (e.g. [23]) or domain-specific designs (e.g. traffic control [24] and manufacturing [25]). Drawing inspiration from both natural and artificial domains, the Multi-Scale Feedbacks (MSF) design pattern was proposed to offer a generic, reusable solution to control scalability problems across various contexts [7]. Hence, goal-oriented, multi-scale self-adaptation solutions (e.g. [26, 22]) combine goal-orientation – for enabling new self-adaptation behaviours to be identified during runtime; with multi-scale designs – for ensuring the scalability of self-adaptation processes.

4. Systems Engineering Enablers

Traditional systems engineering processes such as the one mentioned above used to be mostly supported by natural language documents or at best structured documents such as spreadsheets. Given the increasing complexity of systems, this turned out to be unmanageable to build today's systems at affordable costs. This triggered the development of the Model-Based System Engineering paradigm, where natural language documents are replaced by models of Domain-Specific Modelling Languages (DSML).

Models have been used for a long time to help us understand and analyse complex systems, processes, or artefacts that we are studying, interacting with, managing or developing (e.g. geographical maps, construction blueprints). They are abstractions of reality built for particular purposes [27, 28]. Representing a simplified reality, a model is easier to process than the real thing. However, the way in which a model abstracts reality must be carefully chosen according to the model's purpose. For example, a road map will abstract the land as a set of two dimensional lines indicating road paths so that people can find their way to go from one place to another.

To be usable, models must be understandable in some way. Hence, models must be expressed in some modelling language (e.g. the map's legend) that must be known to understand the models. Such modelling languages can be specified using dedicated metalanguages such as meta-models or grammars. Being expressed in terms of formally specified modelling languages, models can be analysed with tools to automatically detect errors in the system early, which is not possible when only natural language documents are used.

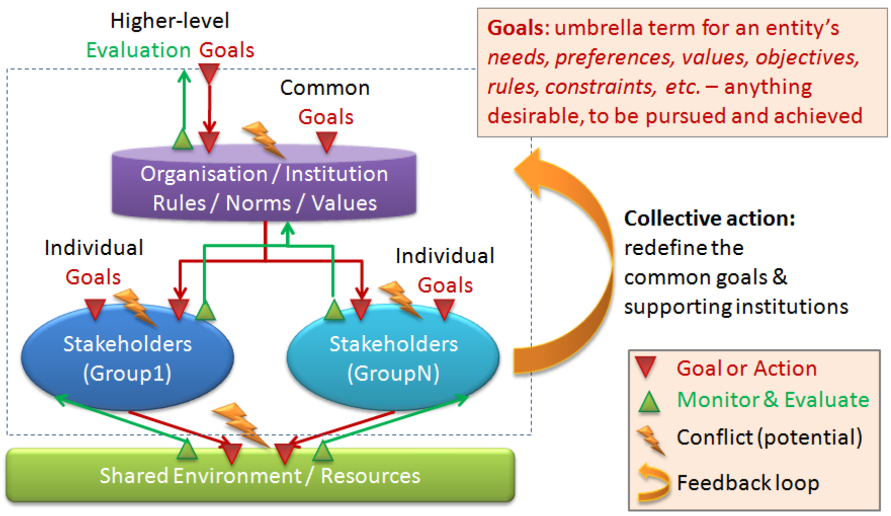

Figure 4: Goal-oriented multi-scale architecture for socio-technical systems

Applied to developing Cyber-Physical Systems (CPS) such Model-Based Engineering paradigm was proven effective leading to better system quality and important cost savings [29]. Besides providing model analysis capabilities, modelling languages also provide a common understanding of the domain intended to be covered by the language. This is achieved through a set of precise concepts and their relationships that formally specify the language and can be used to constitute a common vocabulary for domain actors. It has been shown that expressing something in terms of a properly constructed Domain-Specific Modelling Language (DSML) greatly helps in reducing risks of imprecision, miss-communication and inconsistencies, compared to using natural language. As pointed out in [30], by definition a model is always precise, since its vocabulary is formally defined through a modelling language, being at least precise enough to be understood by computer programs independently of the level of abstraction of the represented reality.

An issue when using such DSMLs is that while expressiveness increases with the specificity of the language, what can be expressed using the language is limited to the covered domain (scope). Therefore, several DSMLs must often be used conjointly to cover all required domains. This observation leads to Multi-Paradigm Modelling (MPM) [31, 4, 32, 33, 34], which advocates the use of a set of modelling languages, each one being most appropriate for the particular subset of activities to be performed with models of the language, rather than trying to build a single monolithic language to support all activities. In particular, Multi-Paradigm Modelling builds upon the following principles:

- Model each part and aspect of a system explicitly, so as to capture all relevant information in terms of formal languages that can be understood and processed by computers;
- Model at the appropriate level(s) of abstraction (or scales) using the most appropriate formalism to avoid introducing accidental complexity.

While the main asset of MPM is to tackle the multi and heterogeneous aspects of systems, it comes at the expense of needing to properly combine them. This is a research topic in its own — model management — where the set of employed models, their modelling languages and the relationships between the models are also formally specified with dedicated DSMLs [33, 35, 36]. Thanks to MPM, language extensibility is supported by allowing the integration of new languages configured for project or organisation-specific needs.

5. Our Approach

Inspired by model-based approaches and paradigms that were successful for Cyber-Physical Systems (as presented earlier) and considering the previously identified commonalities between system engineering and policy making processes, and the commonalities between goal-oriented multi-scale control systems and STSs, we propose to develop a conceptual framework that better supports existing and new policy-making processes specification and application. Such conceptual framework will rely on a set of combined DSMLs and associated tools, to help specify, analyse and understand policy-driven STSs. This will help to detect missing, misapplied or outdated policies; as well as simulate and predict specific effects of various policy updates. This approach will be based on MPM– to benefit from its modelling assets and model integration capabilities.

5.1. Multi-Paradigm Modelling for Socio-Technical Systems

Following MPM principles, we will reuse, adapt, develop and combine the most appropriate modelling languages to cover all aspects of STSs including their policy making processes, as relevant for the modelling activities to be performed at the appropriate abstraction levels. This will provide a precise, shared vocabulary for the policy-making domain, which is already an improvement (compared to using only natural language documents) as it helps to avoid misunderstandings among project stakeholders. For instance, looking at the policy making approach specified in the ETF document [14], we believe that expressing the presented notions and their relationships formally with an appropriate modelling language (ontology) would enforce making the underlying knowledge more explicit and help developing tools to better support the ETF processes.

Reusing or adapting existing modelling languages instead of reinventing new ones can be very beneficial to policy making by taking advantage of knowledge gained in other domains that experienced similar problems. In particular, for the problem identification and policy formulation phases of the policy making process of Fig. 1, policy makers can benefit from the extensive work of the RE community and in particular its aforementioned GORE approaches. For this, we intend to reuse as much as possible existing GORE languages and tools such as the User Requirements Notation (URN)[2], which incorporates a large part of the i* language and approach [17] to capture and analyse goals, stakeholders, their conflicts, resources and so on. Besides, we will benefit from its use case maps sub-language, which allows specification of use case scenario at a high level of abstraction for early policy making phases, and from its goal-oriented decision making methodology based on Key Performance Indicators (KPI) [37]. Thanks to its jUCMNav tool[3] supporting these features, several analyses to evaluate KPIs can easily be developed and evaluated from goal models. In addition, use case scenarios can be simulated with the built-in simulator to detect inconsistency in system behaviour early, thanks to a simple action language. Several benefits of using this tool early have been shown in [30], among others.

Furthermore, existing successful solutions for adaptation management in complex CPSs will be extended and customised to bring some of the necessary support to modern policy-driven STSs. A starting point will be to propose a DSML to represent, analyse and understand policy-driven adaptations for the specific STS domain (e.g. forestry management, co-design of shared living spaces). Coupled with the aforementioned goal models using MPM, the language will support modelling goal-oriented, multi-scale architectures for controlling complex STSs (e.g. smart homes and power grids [26, 38]), Fig. 4. Here, *goals* are first-class system entities, representing anything that a system is willing to achieve or enforce – e.g. objectives, values, constraints, rules, policies, norms, priorities, actions. Each goal is defined by: i) a specific *evaluation function*, defining how to assess goal achievement; and ii) a *spatio-temporal scope*, defining where and when to achieve the goal.

[2]URN: https://www.itu.int/rec/T-REC-Z.151/en/
[3]jUCMNav: http://softwareengineering.ca/jucmnav/

A system may pursue several goals simultaneously. Goals may be in *conflict* if they pursue incompatible objectives over intersecting spatio-temporal scopes. A continuous control feedback loop aims to achieve each system's goal, based on internal resources and the external context. To reach a system goal, such control loop may aim to achieve 'lower-level' goals first, and so forth, recursively. This leads to a multi-scale organisation of control loops, which run simultaneously and coordinate to achieve goals and manage conflicts.

Modelling complex systems in this manner helps preliminary analysis at design time – by rendering goals, system controllers and relevant context aspects explicit and allowing to detect conflicts and/or tune controllers accordingly. It also becomes essential for system adaptation at run-time, when dynamic changes occur – e.g. detecting new conflicts and adapting controllers to resolve them, when new goals or resources are added-on. The goal-oriented aspect contrasts traditional control approaches based on predefined rules and static system models, which could not adapt to unforeseen changes. The multi-scale design also helps manage system complexity, by abstracting system concepts at different scales and hiding irrelevant details from the scales below – hence applying a divide-and-conquer technique that limits the amount of resources necessary at each scale [39].

We believe that applying these concepts and modelling technique to policy-driven STSs will help formalise policy-management processes and render them more traceable and rational. It will help, for instance: to identify all system goals (objectives, policies, values, constraints, etc); to analyse and identify potential conflicts; to detect missing, misapplied or ineffective policies; and, to simulate some of the effects of various policy changes. Providing a multi-scale design also matches the current structure of most political institutions, where the aforementioned processes may run simultaneously, while dealing with cross-scale conflicts and synchronisation issues. Existing knowledge from cross-domain multi-scale control systems may also be useful here, to better understand and manage such multi-scale policy-making processes.

In order to better guide users in following adopted policy-making processes such as the one depicted by Figs. 1 and 2, our framework will also allow modelling these processes using standard workflow models and tools, adapted to the needed modelling activities, similar to what is proposed in [40, 34]. By guiding stakeholders in performing their modelling and analysis activities thanks to these workflows, we can propose more advanced automatic tools for problem detection, solution proposals and impact predictions. For instance, more sophisticated simulations may be proposed via agent-based modelling (ABM) relying on existing platforms – e.g., Repast[4] (social sciences), GAMA[5] (spatially-aware agents), SARL[6] (holonic agents); NetLogo[7] (general-purpose entry-level ABM platform), JADE[8]. In particular, if other simulating tools are found beneficial, we will use MPM co-simulation approaches [41] to coordinate existing simulators and improve simulation by integrating different paradigms.

[4]Repast: https://repast.github.io

[5]GAMA: https://github.com/gama-platform

[6]SARL: http://www.sarl.io

[7]NetLogo: https://ccl.northwestern.edu/netlogo

[8]JADE: https://jade-project.gitlab.io/

5.2. Assumptions, Threats and Limitations

While promising, and despite the observed similarities between complex CPSs (including human actors) and STSs, our approach relies on several assumptions that can only be verified by pursuing the proposed research direction, developing associated tools and applying them to policy making in various real-world STSs. We discuss these assumptions and how they can be mitigated below.

The main question is whether what worked for CPS can also work, at least partially, for STSs. Regarding DSMLs, developing formal ontologies for certain domains has proven rather tedious a process, due to the difficulty in converging on a single set of commonly-accepted domain concepts. For instance, for the CPS domain, modelling languages such as AADL[9] have been developed for more than 15 years. However, mitigating this threat, we note that this situation did not prevent approaches and tools from being developed early-on during the language specification, allowing benefits to be obtained right from the incipient phases. This is also the case for programming languages. For example, discussing the appropriateness of one language over another often leads to long debates without resolution. What matters is that DSMLs, even if imperfect, can already bring benefits.

Besides, while DSML development is a complicated, iterative process, approaches such as [42] exist to take into account users and usage context at the very beginning of DSML development. This will help ensure that the targeted stakeholders, such as policy makers (often with social science backgrounds), will be able to use modelling processes and tools despite their differences from typical model and tools users with engineering backgrounds.

We must also consider the fact that the proposed modelling and analysis processes would be carried-out by human actors (rather than automatic agents) and within open socio-technical contexts (rather than constrained environments that can be completely formalised and controlled). Hence, we aim to make sure that the provided modelling platform offers sufficient flexibility and expressiveness to suit complex unforeseen socio-technical situations; and avoid over-constraining and pre-formatting all possible system representations. Indeed, our intention is to provide a helpful tool, rather than a limiting control framework. Thus, we will ensure that actors can easily extend or update the underlying languages and tools to express exceptional cases and diverse view-points.

Another important aspect is that this proposal can only provide support for achieving well-defined goals, in conformity with well-established societal values. While it can allow actors to change and evolve their goals over time, it provides no magic solution against conflicting goals, misaligned values or lack of political will for systemic change.

Finally, we hope that substantial gain from modelling can be achieved by providing a common vocabulary, facilitating understanding and encouraging better precision in policy specifications; and by providing better support for policy analyses, including simulation. Such benefits must be sufficiently significant to overcome the overheads involved in learning new tools and modelling processes.

[9] AADL: http://www.aadl.info/

6. Related Work on Policy-Making Tools for Socio-Technical Systems

To our knowledge, there has been limited efforts to provide policy-making support tools. For instance, we note the GRACeFUL project (Global systems Rapid Assessment tools through Constraint Functional Languages)[10], which aims to develop smart tools that guide decision makers during the implementation of urban projects. The main objective of this project was to develop a simulation platform for modelling the possible responses of citizens and other stakeholders involved, so that the tool can generate predictions from multiple view-points about various policy implementations. Similar to our approach, one concern of the project was to make this kind of modelling accessible to nonspecialists. This was achieved apparently via a graphic platform that facilitated the development of custom software tools.

We plan to achieve similar advantages with our approach, while adopting MPM at the heart of our language engineering, tool building and model integration processes. Still, while the focus of GRACeFUL was on functional languages, where policy making is seen as a constraints-solving problem, our contribution is considerably wider. It aims to develop not only the decision making support tools but also to establish the necessary foundations and conceptual framework for the policy-making domain; and enable these to be customised and extended for various application domains and project requirements. Moreover, we believe that the policy-making domain will be better addressed by a combination of paradigms rather than by a single one (constraints solving).

Regarding process modelling, [43] investigated the feasibility of using workflow tools to support policy-making processes. It presents lessons learned from cases in four European countries and concludes that the processes show several commonalities (common tasks and sequence of steps) despite that they belong to different policy domains. The authors also identify a lack of any supporting information technology, which prevents transparency in policy making processes. These are shortcomings that our proposal aims to address.

7. Conclusion and Future Work

This position paper identified the need for more formal support in policy-making processes, to help policy-makers deal with inherent complexities: identifying and considering the multiple stakeholders, objectives and viewpoints relevant to the specified policies; taking into account the diverse facets to be managed in the targeted application domain (via the specified policies); understanding the potential effects of policy updates and interpreting the observable effects of existing policies upon their application domains. Drawing inspiration from successful solutions to similar problems in technical systems (e.g. CPS), we propose to develop a conceptual modelling framework and support tools to help such policy-making processes. We rely on our previous experience with: i) domain-specific modelling languages and multi-paradigm modelling; and ii) goal-oriented multi-scale architectures for complex self-adaptive systems. We aim to extend and adapt relevant solutions available from these areas to address the particular challenges of the policy-making domain, within the socio-technical systems context. We believe that

[10]GRACeFUL: http://www.fetfx.eu/project/graceful/

such modelling framework, even if necessarily imperfect and continuously evolving, would provide essential support for improving the efficacy, efficiency, comprehension and traceability of policy-making processes.

References

[1] J. M. Barrutia, C. Echebarria, M. R. Paredes, P. Hartmann, V. Apaolaza, From rio to rio+20: twenty years of participatory, long term oriented and monitored local planning?, Journal of Cleaner Production 106 (2015) 594–607.

[2] P. Lalanda, C. Hamon, An autonomic mediation framework for complex physical environments, in: 2014 IEEE International Congress on Big Data, Anchorage, AK, USA, June 27 - July 2, 2014, IEEE Computer Society, 2014, pp. 506–513. URL: https://doi.org/10.1109/BigData.Congress.2014.80. doi:10.1109/BigData.Congress.2014.80.

[3] I. Errandonea, S. Beltrán, S. Arrizabalaga, Digital twin for maintenance: A literature review, Comput. Ind. 123 (2020) 103316. URL: https://doi.org/10.1016/j.compind.2020.103316. doi:10.1016/j.compind.2020.103316.

[4] M. Amrani, D. Blouin, R. Heinrich, A. Rensink, H. Vangheluwe, A. Wortmann, Multi-paradigm modelling for cyber–physical systems: a descriptive framework, Software and Systems Modeling 20 (2021). doi:10.1007/s10270-021-00876-z.

[5] S. Kounev, P. R. Lewis, K. L. Bellman, N. Bencomo, J. Cámara, A. Diaconescu, L. Esterle, K. Geihs, H. Giese, S. Götz, P. Inverardi, J. O. Kephart, A. Zisman, The notion of self-aware computing, in: S. Kounev, J. O. Kephart, A. Milenkoski, X. Zhu (Eds.), Self-Aware Computing Systems, Springer International Publishing, 2017, pp. 3–16.

[6] P. Lalanda, J. A. McCann, A. Diaconescu, Autonomic Computing - Principles, Design and Implementation, Undergraduate Topics in Computer Science, Springer, 2013. URL: https://doi.org/10.1007/978-1-4471-5007-7. doi:10.1007/978-1-4471-5007-7.

[7] A. Diaconescu, L. J. D. Felice, P. Mellodge, Exogenous coordination in multi-scale systems: How information flows and timing affect system properties, Future Gener. Comput. Syst. 114 (2021) 403–426. URL: https://doi.org/10.1016/j.future.2020.07.034. doi:10.1016/j.future.2020.07.034.

[8] R. B. France, B. Rumpe, Model-driven development of complex software: A research roadmap, CoRR abs/1409.6620 (2014).

[9] K. L. B. et al., Self-improving system integration: Mastering continuous change, Future Gener. Comput. Syst. 117 (2021) 29–46. URL: https://doi.org/10.1016/j.future.2020.11.019. doi:10.1016/j.future.2020.11.019.

[10] J. Wilkes-Allemann, A. Ludvig, S. Gobs, E. Lieberherr, K. Hogl, A. Selter, Getting a grip on negotiation processes: Addressing trade-offs in mountain biking in austria, germany and switzerland, Forest Policy and Economics 136 (2022) 102683. URL: https://www.sciencedirect.com/science/article/pii/S1389934121002896. doi:https://doi.org/10.1016/j.forpol.2021.102683.

[11] G. Weiss, E. Hansen, A. Ludvig, E. Nybakk, A. Toppinen, Innovation governance in the forest sector: Reviewing concepts, trends and gaps, Forest Policy and Economics 130

(2021) 102506. URL: https://www.sciencedirect.com/science/article/pii/S138993412100112X. doi:https://doi.org/10.1016/j.forpol.2021.102506.

[12] A. Ludvig, M. Braun, F. Hesser, L. Ranacher, D. Fritz, T. Gschwantner, R. Jandl, G. Kindermann, T. Ledermann, W. Pölz, K. Schadauer, B. F. Schmid, C. Schmid, P. Schwarzbauer, G. Weiss, B. Wolfslehner, P. Weiss, Comparing policy options for carbon efficiency in the wood value chain: Evidence from austria, Journal of Cleaner Production 292 (2021) 125985. URL: https://www.sciencedirect.com/science/article/pii/S0959652621002055. doi:https://doi.org/10.1016/j.jclepro.2021.125985.

[13] S. Long, Socioanalytic Methods: Discovering the Hidden in Organisations and Social Systems, Karnac Books Limited, 2013. URL: https://books.google.fr/books?id=LWL7krX7jgAC.

[14] Madlen Serban, Supporting Public Policy Making through Policy Analysis and Policy Learning , Technical Report, European Training Foundation, 2015. doi:10.2816/721877.

[15] E. Lee, The past, present and future of cyber-physical systems: A focus on models, Sensors 15 (2015) 4837–4869. URL: http://dx.doi.org/10.3390/s150304837. doi:10.3390/s150304837.

[16] D. Nunes, J. S. Silva, F. Boavida, A Practical Introduction to Human-in-the-Loop Cyber-Physical Systems, Wiley, 2018. URL: https://www.wiley.com/en-us/A+Practical+Introduction+to+Human+in+the+Loop+Cyber+Physical+Systems-p-9781119377788.

[17] E. Yu, N. Giorgini, Paola anb Maiden, J. Mylopoulos, Social Modeling for Requirements Engineering, MIT Press, 2011.

[18] A. Dardenne, A. van Lamsweerde, S. Fickas, Goal-directed requirements acquisition, Science of Computer Programming 20 (1993) 3–50. URL: https://www.sciencedirect.com/science/article/pii/016764239390021G. doi:https://doi.org/10.1016/0167-6423(93)90021-G.

[19] A. I. Antón, C. Potts, The use of goals to surface requirements for evolving systems, in: Proceedings of the 20th International Conference on Software Engineering, ICSE ’98, IEEE Computer Society, USA, 1998, p. 157–166.

[20] J. Horkoff, F. Aydemir, E. Cardoso, T. Li, A. Maté, E. Paja, M. Salnitri, L. Piras, J. Mylopoulos, P. Giorgini, Goal-oriented requirements engineering: an extended systematic mapping study, Requirements Engineering 24 (2019). doi:10.1007/s00766-017-0280-z.

[21] R. P. Würtz (Ed.), Organic Computing, Understanding Complex Systems, Springer, 2008.

[22] A. Diaconescu, S. Frey, C. Müller-Schloer, J. Pitt, S. Tomforde, Goal-oriented holonics for complex system (self-)integration: Concepts and case studies, in: G. Cabri, G. Picard, N. Suri (Eds.), 10th IEEE International Conference on Self-Adaptive and Self-Organizing Systems, SASO 2016, Augsburg, Germany, September 12-16, 2016, IEEE Computer Society, 2016, pp. 100–109.

[23] H. A. Simon, The architecture of complexity, in: Facets of systems science, Springer, 1991, pp. 457–476.

[24] K. Fischer, Holonic multiagent systems – theory and applications, in: P. Barahona, J. J. Alferes (Eds.), Progress in Artificial Intelligence, Springer Berlin Heidelberg, Berlin, Heidelberg, 1999, pp. 34–48.

[25] M. Ulieru, R. A. Este, The holonic enterprise and theory emergence: On emergent features of self-organization in distributed virtual agents, Cybern. Hum. Knowing 11 (2004) 79–98.

[26] S. Frey, A. Diaconescu, D. Menga, I. M. Demeure, A generic holonic control architecture for heterogeneous multiscale and multiobjective smart microgrids, ACM Trans. Auton. Adapt.

Syst. 10 (2015) 9:1–9:21. URL: https://doi.org/10.1145/2700326. doi:10.1145/2700326.
[27] J. Rothenberg, The Nature of Modeling, John Wiley & Sons, Inc., USA, 1989, p. 75–92.
[28] B. Combemale, R. France, J.-M. Jezequel, B. Rumpe, J. Steel, D. Vojtisek, Engineering Modeling Languages - Turning Domain Knowledge into Tools, Chapman and Hall/CRC, 2017.
[29] J. Hansson, S. Helton, P. Feiler, ROI Analysis of the System Architecture Virtual Integration Initiative, Technical Report CMU/SEI-2018-TR-002, Software Engineering Institute, Carnegie Mellon University, Pittsburgh, PA, 2018. URL: http://resources.sei.cmu.edu/library/asset-view.cfm?AssetID=517157.
[30] D. Blouin, H. Giese, Combining requirements, use case maps and aadl models for safety-critical systems design, in: 2016 42th Euromicro Conference on Software Engineering and Advanced Applications (SEAA), 2016, pp. 266–274. doi:10.1109/SEAA.2016.15.
[31] H. Vangheluwe, J. de Lara, P. Mosterman, An introduction to multiparadigm modelling and simulation, in: Proceedings of the AIS'2002 Conference 9–20 (2002). 35, Press, 2002.
[32] D. Blouin, R. Al-Ali, M. Iacono, B. Tekinerdogan, H. Giese, Chapter 2 - an ontological foundation for multi-paradigm modelling for cyber-physical systems, in: B. Tekinerdogan, D. Blouin, H. Vangheluwe, M. GoulÃ£o, P. Carreira, V. Amaral (Eds.), Multi-Paradigm Modelling Approaches for Cyber-Physical Systems, Academic Press, 2021, pp. 9–43. URL: https://www.sciencedirect.com/science/article/pii/B9780128191057000076. doi:https://doi.org/10.1016/B978-0-12-819105-7.00007-6.
[33] H. Giese, D. Blouin, R. Al-Ali, H. Mkaouar, S. Bandyopadhyay, M. Iacono, M. Amrani, S. Klikovits, F. Erata, Chapter 4 - an ontology for multi-paradigm modelling, in: B. Tekinerdogan, D. Blouin, H. Vangheluwe, M. GoulÃ£o, P. Carreira, V. Amaral (Eds.), Multi-Paradigm Modelling Approaches for Cyber-Physical Systems, Academic Press, 2021, pp. 67–122. URL: https://www.sciencedirect.com/science/article/pii/B978012819105700009X. doi:https://doi.org/10.1016/B978-0-12-819105-7.00009-X.
[34] D. Blouin, R. Al-Ali, H. Giese, S. Klikovits, S. Bandyopadhyay, A. BariÅ¡iÄ‡, F. Erata, Chapter 5 - an integrated ontology for multi-paradigm modelling for cyber-physical systems, in: B. Tekinerdogan, D. Blouin, H. Vangheluwe, M. GoulÃ£o, P. Carreira, V. Amaral (Eds.), Multi-Paradigm Modelling Approaches for Cyber-Physical Systems, Academic Press, 2021, pp. 123–145. URL: https://www.sciencedirect.com/science/article/pii/B9780128191057000106. doi:https://doi.org/10.1016/B978-0-12-819105-7.00010-6.
[35] D. Blouin, Y. Eustache, J.-P. Diguet, Extensible global model management with meta-model subsets and model synchronization, in: GEMOC@MoDELS, 2014.
[36] T. Beyhl, R. Hebig, H. Giese, A model management framework for maintaining traceability links, in: Software Engineering, 2013.
[37] A. Pourshahid, I. Johari, G. Richards, D. Amyot, O. Akhigbe, A goal-oriented, business intelligence-supported decision-making methodology, Decision Analytics 1 (2014). doi:10.1186/s40165-014-0009-8.
[38] A. Diaconescu, J. Pitt, Holonic institutions for multi-scale polycentric self-governance, in: A. Ghose, N. Oren, P. R. Telang, J. Thangarajah (Eds.), Coordination, Organizations, Institutions, and Norms in Agent Systems X - COIN 2014 International Workshops, COIN@AAMAS, Paris, France, May 6, 2014, COIN@PRICAI, Gold Coast, QLD, Australia, December 4,

2014, Revised Selected Papers, volume 9372 of *Lecture Notes in Computer Science*, Springer, 2014, pp. 19–35.

[39] A. Simon, The architecture of complexity, in: Proceedings of the American Philosophical Society 106, 1962, pp. 467–482.

[40] L. Lúcio, S. Mustafiz, J. Denil, H. Vangheluwe, M. Jukss, FTG+PM: An Integrated Framework For Investigating Model Transformation Chains, in: International SDL Forum, 2013, pp. 182–202.

[41] C. Gomes, C. Thule, D. Broman, P. G. Larsen, H. Vangheluwe, Co-simulation: A survey, ACM Computing Surveys 51 (2018) 49.

[42] A. Barišić, D. Blouin, V. Amaral, M. Goulão, A requirements engineering approach for usability-driven dsl development, in: Proceedings of the 10th ACM SIGPLAN International Conference on Software Language Engineering, SLE 2017, Association for Computing Machinery, New York, NY, USA, 2017, p. 115–128. URL: https://doi.org/10.1145/3136014.3136027. doi:10.1145/3136014.3136027.

[43] V. Weerakkody, H. Lee, A. Ko, T. D. Medeni, R. El-Haddadeh, A. Tsohou, K. Al-Yafi, Z. Irani, L. M. Campos, Supporting public policy making processes with workflow technology: Lessons learned from cases in four european countries, Int. J. Electron. Gov. Res. 8 (2012) 63–77. URL: https://doi.org/10.4018/jegr.2012070104. doi:10.4018/jegr.2012070104.

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A Multiparadigm Modeling Investigation of Membrane Chemical Degradation in PEM Fuel Cells

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We report a multi-paradigm model of the membrane chemical degradation in Polymer Electrolyte Membrane Fuel Cells (PEMFCs), by combining Coarse-Grained Molecular Dynamics (CGMD) and a multiscale cell performance model. CGMD is used to generate structural databases that relate the amount of detached (degraded) ionomer sidechains with the water content and the resulting PEM meso-microporous structure. The multiscale cell performance model describes the electrochemical reactions and transport mechanisms occuring in the electrodes from an on-the-fly coupling between Kinetic Monte Carlo (KMC) sub-models parametrized with Density Functional Theory (DFT) data and (partial differential equations-based) continuum sub-models. Furthermore, the performance model includes a kinetic PEM degradation sub-model which integrates the CGMD database. The cell model also predicts the instantaneous PEM sidechain content and conductivity evolution at each time step. The coupling of these diverse modeling paradigms allows one to describe the feedback between the instantaneous cell performance and the intrinsic membrane degradation processes. This provides detailed insights on the membrane degradation (sidechain detachment as well as water reorganization within the PEM) during cell operation. This novel modeling approach opens interesting perspectives in engineering practice to predict materials degradation and durability as a function of the initial chemical composition and structural properties in electrochemical energy conversion and storage devices.

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From the second half of the twentieth century, Polymer Electrolyte Membrane Fuel Cells (PEMFCs) have attracted much attention due to their potential as a clean power source for vehicles traction. Market introduction of FC vehicles is being recognized of highest priority in many developed countries due to their impact on the reduction of energy consumption and greenhouse gas emissions. However, PEMFC technologies have not yet reached all the requirements to be competitive, in particular regarding their high production cost of Membrane Electrode Assemblies and their low durability.

Indeed, meso/micro-structural degradation leading to the PEMFC components aging is attributed to several complex physicochemical mechanisms not yet completely understood. The associated components meso/micro-structural changes translate into irreversible long-term cell power degradation.[1–3] For instance, dissolution and redistribution of the catalyst reduces the specific catalyst surface area and the electrochemical activity. The corrosion of the catalyst carbon-support and loss or decrease of the hydrophobicity caused by an alteration of the Polytetrafluoroethylene in Catalyst Layers (CLs), Microporous Layers and Gas Diffusion Layers also affect the water management in the cell and thus the electrochemical performance.

Regarding the polymer electrolyte in PEMFCs, a large number of materials has been tested, including sulfonated hydrocarbon polymers, phosphoric acid doped polybenzimidazole, polymer-inorganic composite membranes or solid acid membranes. However, the most widely used are still the PerFluoroSulfonated Acid (PFSA) polymers (the so-called Nafion from DuPont, Figure 1). Apart from mechanical degradations such as thinning and pinhole formations,[4] chemical and electrochemical degradations can take place in the PFSA-based membranes and in the ionomer inside the CLs.[5]

Significant permeation of the reactants across PEM, in particular oxygen from the cathode to the anode, has been often experimentally reported as being the major cause of PEM chemical degradation.[6–8] The formation of hydrogen peroxide (H_2O_2) at the anode CL[9,10] is attributed to the following reaction

$$H_2 + O_2 \rightarrow H_2O_2 \quad [1]$$

Formation of H_2O_2 may also occur at the cathode CL as part of the Oxygen Reduction Reaction (ORR),

$$O_2 + 2\,H^+ + 2\,e^- \rightarrow H_2O_2 \quad [2]$$

in particular if Pt-M catalysts are used, with M being a transition metal element.[11]

H_2O_2 is a highly oxidizer reagent which may deteriorate the PEM. Furthermore, PEM degradation leads to an increasing reactants crossover between the CLs. Young et al. reported that at non-zero current densities a performance decay is observed due to an increase of the PEM resistance, that is, a decrease of the PEM conductivity.[12] As this conductivity is directly related to the side chains presence, it was concluded that the radical reaction responsible of the chemical degradation involves not only an attack on the backbone but on the side

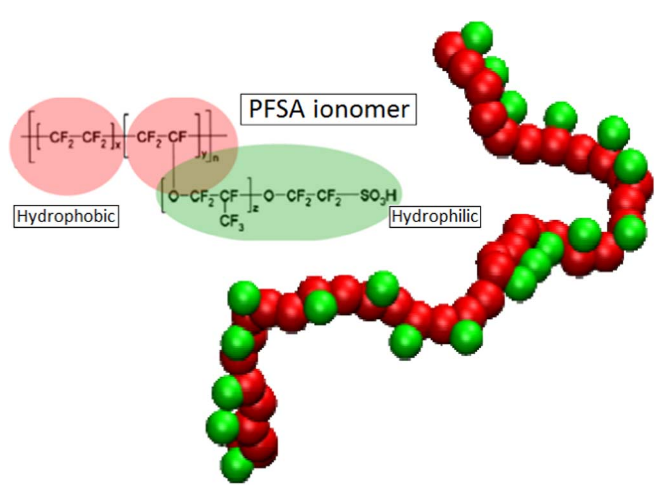

Figure 1. Representation of our Coarse Grain Nafion model in which the hydrophobic backbone is replaced by a coarse-grained chain of 20 apolar beads (red color) and the entire side chain is replaced by a negatively charged bead (green color).

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chain as well (mechanism known as side chain unzipping). Other experiments demonstrated that in particular Open Circuit Voltage (OCV) conditions are strongly damageable for the PEM.[13–15]

One of the key factors enhancing the PEM chemical degradation is the presence of Fenton's ions (for example Fe^{2+} or Cu^{2+}) in the cell which will initiate the decomposition of H_2O_2 into radicals OH° and OOH°.[16–19] The most plausible origins of these ions are the degradation of iron containing end-plates which are used in the PEMFCs, and the oxidation of the pipes in the reactants management system.[20,21] Additionally, some debate still remains about the role of the precipitated Pt (arising from electrochemical dissolution mainly in the cathode CL) on catalyzing the H_2O_2 decomposition.[22,23] Interestingly, some of the PEM degradation products were reported to contaminate the catalyst and decrease its ORR activity within the CLs.[24]

Numerous mathematical models have been developed with the aim to understand the large diversity of experimental observations.[25] For instance, Xie and Hayden originally proposed a continuum kinetic model describing the chemical degradation of the PEM as function of the concentrations of radicals OH° and OOH°.[26] Their model is based on the *unzipping mechanism* where backbone and side chains are cutted starting from sites containing impurity carboxylic groups. Significant concentrations for these groups have been reported in earlier versions of Nafion.[27] The carboxylic acid groups are either direct by-product of the PEM synthesis or the result of reactions of other contaminants with radical species. This carboxylic acid reacts with the two radicals OH° and OOH°. Carbon dioxide and HF are then released and the carboxylic acid group is transformed into a fluoride acid group which is then hydrolyzed, releasing another HF molecule and regenerating the carboxylic acid group.[28] After each degradation step, the PEM backbone loses one carbon atom. Besides, Ishimoto et al. performed density functional theory (DFT) calculations to understand the chemical degradation mechanism of side chains by hydroxyl radical attacks.[29] The energy profiles from these DFT calculations have supported the reaction mechanism proposed by Xie and Hayden.[26]

Chen and Fuller proposed a continuum H_2O_2 formation model based on a CL agglomerate approach.[30] They simulated the production of H_2O_2 at the anode and at the cathode through chemical and electrochemical pathways. The H_2O_2 formation model is coupled to an oxygen permeation model, and validated with experimental data. However the impact of the H_2O_2 formation on the PEM degradation is not described and thus the cell potential decay over time is not calculated. Others reported continuum models describing the H_2O_2 decomposition, the radicals formation and the ionomer degradation,[31] but still without predicting the induced cell performance decay over time. Shah et al. proposed a Continuum Fluid Dynamics (CFD) model accounting for the PEM degradation, water transport and thermal management within a pre-existing cell model.[32] In their model, they ignore the side chain unzipping mechanism, which means that a constant conductivity of the PEM is assumed, and thus the effect of the degradation on the transport phenomena and the cell performance cannot be captured.

Additionally, some recent molecular dynamics (MD) works have been reported predicting that the presence of ferric ions may affect the intrinsic PEM proton transport properties.[33]

We reported the first models aiming at account for the instantaneous feedback between the PEM chemical degradation and the electrochemical and transport processes in a PEMFC.[2,34–37] The approach behind these models treats PFSA PEMs with a structure influenced by humidification, which also impacts the local transport properties of mass and charge within the PEM. In order to study the PEM degradation, a multi-species transport model is used for protons, water, dissolved gases, radicals, and ions. This model includes detailed chemical reaction mechanisms of hydrogen peroxide formation, hydrogen peroxide decomposition, and radical attack of the PEM. A numerical feedback between degradation, mesostructure, and performance is established, allowing predicting the potential decay associated to the membrane degradation process. The mesostructural parameters considered are the PEM average porosity and tortuosity, evolving with the (degrading) side chains concentration. In our approach the effective porosity is defined macroscopically as the water volume fraction which is assumed to be

$$\varepsilon = \frac{\lambda}{\lambda + \frac{\bar{V}_{Nafion}}{\bar{V}_{H_2O}}} \quad [3]$$

where ε refers to the effective porosity (defined as the water volume fraction), λ to the water content (number of water molecules per sulfonic acid group), $\bar{V}_{Nafion}$ to the partial molar volume fraction of PEM and $\bar{V}_{H_2O}$ to the partial molar volume fraction of water. $\bar{V}_{Nafion}$ is assumed to be related to the PEM equivalent weight through the expression

$$\bar{V}_{Nafion} = \frac{EW}{\rho_{dry}} = \frac{1}{\left((1+s\lambda)^3 c_{\text{side chains}}\right)} \quad [4]$$

where s is the swelling factor of the membrane and $c_{\text{side chains}}$ the concentration of side chains calculated through a kinetic degradation model. Then, the variation of the membrane conductivity with the effective porosity is calculated through the mean field expression proposed by Choi et al.[38,39]

$$g_{H^+} = \frac{\varepsilon}{\tau}\left[\frac{F^2}{RT}\left(D^{\Sigma}_{H^+}\cdot C^{\Sigma}_{H^+} + D^{G}_{H^+}\cdot C_{H^+} + D^{E}_{H^+}\cdot C_{H^+}\right)\right] \quad [5]$$

where the tortuosity toward the proton transport τ is function of the effective porosity through the Prager's model.[34] Based on our previous approach, Wong and Kjeang recently reported continuum models predicting how the cell operation conditions impact the PEM degradation kinetics, albeit by disregarding the PEM degradation effects on potential decay.[40,41] Similar remark can be done for a recent work on PEM Water Electrolyzers, also based on our approach.[42]

Despite the insights provided by these modeling efforts there is still a lack of modeling approach being able to investigate the influence of the chemical degradation kinetics on the meso/micro-structural properties of the PEM at the molecular level. As well, the retroactive impact of the PEM meso/microstructure evolution on the instantaneous performance and durability of a PEMFC as function of the applied operation conditions on the cell deserves further investigations.

At the meso/microsopic scale, interactions between molecular components control the processes of structural formation which lead to random phase-segregated morphologies in PEMs and CLs. Such complex processes can be studied by coarse-grained molecular dynamics (CGMD) simulations.[43–45] Complex morphologies of the emerging media can be related to relevant effective properties that characterize transport and reaction, using concepts from the theory of random heterogeneous media. Finally, conditions for durable operation at the macroscopic device level can be defined and balance equations for involved species, i.e. electrons, protons, reactant gases and water, can be established on the basis of fundamental conservation relationships. Thereby full relations between structure, properties and performance could be established, which in turn would allow to predict architectures of materials and operating conditions that optimize fuel cell operation.

A significant number of mesoscale computational approaches have been employed to understand the phase-segregated morphology and transport properties of water-swollen Nafion membranes.[46–49] Because of computational limitations, full atomistic models are not able to probe the random morphology of these systems. However, as demonstrated by these simulations and applications to other random composite media, mesoscale models are computationally feasible to capture the morphology. For Nafion, most of these simulations support the idea that narrow water-filled channels and irregularly shaped, nanometer-size clusters of ionic head groups and water forms the proton-conducting network that is embedded into the hydrophobic matrix.

In this paper we report a novel model to analyze PEM degradation and cell performance decay which combines a multi-paradigm, multi-scale cell model with a meso/microstructure resolved PEM

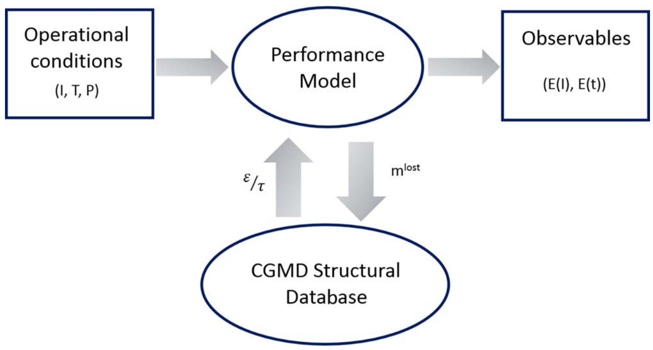

Figure 2. The numerical methodology implemented for the multi-paradigm combination of the multi-scale performance model with the CGMD generated data.

degradation model based on CGMD databases. The technical feasibility of the combination between performance cell models and CGMD databases have been already demonstrated by us for describing carbon corrosion in PEMFC CLs.[50] To the best of our knowledge, we report here the first modeling-based analysis of the PEM meso/microstructure upon its degradation and continuous feedback with the cell performance.

This paper is organized as following. First we present the adopted methodology from CGMD simulations and describe the performance modeling approaches. Then we present structural results and simulation results of performance decay for different simulated operation conditions. Thereafter we conclude and indicate further directions to continue this work.

Overall Methodology

The implemented overall methodology consists on achieving continuous numerical iterations between a performance model (Performance model section) and a PEM meso-structural database extracted from CGMD simulations (CGMD simulations section), as presented in Figure 2. At each numerical iteration, the performance model calculates the instantaneous cell performance and state variables such as the ionomer mass loss due to chemical degradation across the PEM. The performance model retrieves changes on the proton conductivity and the ratio of porosity (ε) over the tortuosity (τ) of the PEM hydrophilic channels from the CGMD-generated database. These structural changes are assumed to be mainly due to chemical degradation, thus, the performance model uses them to correct the mathematical expressions of the proton conductivity as well as diffusion of chemical species across the hydrophilic channels of the PEM following the look-up tables in Equations 6 and 7 here below:

$$\sigma_{H^+}^{eff} = \Omega\,(\%\,\text{SA groups lost}) \qquad [6]$$

$$\frac{\varepsilon}{\tau} = \Phi\,(\%\,\text{SA groups lost}) \qquad [7]$$

with

$$D_i^{eff} = \frac{\varepsilon}{\tau} D_i^0 \qquad [8]$$

In return, the performance evolution of the cell and the structural evolution of the PEM are simultaneously simulated.

As discussed in Introduction section, the mechanism of the chemical attack of the polymer is very complex. It may involve both backbone and side-chain degradation and it is the subject of many debates. Here, we assume that only OH° radicals are the responsible agent of the chemical degradation, and that only the side chains are being attacked. This assumption is consistent with conclusions on modern Nafion obtained by Ghassemzadeh and Holdcroft on the basis of nuclear magnetic resonance (NMR) spectroscopy experiments.[51] Indeed, according to the authors, modern Nafion (e.g. Nafion 211) is chemically stabilized for which the concentration of terminal carboxylic acid groups was decreased to negligible levels[52,53] and thus the backbone remains unaffected by the OH° radicals.

CGMD simulations.— The details of the computational approach based on CGMD simulations are explained elsewhere[43–45,50] and is developed in two major steps. In the first step, Nafion chains, water and hydronium molecules are replaced by corresponding spherical beads with predefined sub-nanoscopic length scale. In the second step, parameters of renormalized interaction energies between the distinct beads are specified.

We consider four main types of spherical beads: polar, nonpolar, apolar, and charged beads.[54] Clusters including a total of four water molecules or three water molecules plus a hydronium ion are represented by polar beads of radius 0.43 nm. The simulation box contained 72 coarse-grained Nafion chains each consisting of 20 monomers and 20 side chains. Each monomeric unit is represented by two apolar beads for backbone (red) and one single polar bead (green) for the entire sidechain (including etheric group) as depicted in Figure 1. We adopted the same coarse graining strategy as in our previous work[44] which was also suggested earlier in Ref. 55. A side chain unit has a molecular volume of 0.306 nm, equivalent to the molecular volume of a four-monomeric unit of polytetrafluoroethylene (PTFE), of size 0.325 nm. Thus in our coarse-graining, a monomeric backbone unit, i.e.,–CF_2–CF_2–CF_2–CF_2–CF_2–CF_2–CF_2–CF_2–, is represented by two beads and a perfluorinated ether sulfonic sidechain is represented by one single bead. Our coarse-graining strategy requires all beads have identical volume set at 0.315 nm^3. The selected box size does not impact the cell performance since the pore structure remains unchanged for box volumes larger than 50 × 50 × 50 nm^3 and we do not expect significant changes in the O_2 crossover or in the proton conductivity.

The interactions between non-bonded beads are modeled by the Lennard-Jones (LJ) potential

$$U_{LJ}(r) = 4D_{ij}^0\left[\left(\frac{r_{ij}}{r}\right)^{12} - \left(\frac{r_{ij}}{r}\right)^{6}\right] \qquad [9]$$

where the effective bead diameter (r_{ij}) is 0.43 nm for side-chain, backbone and water beads. The strength of interaction (D^0) is limited to five possible values ranging from weak (1.8 kJ/mol) to strong (5 kJ/mol) beads.[54] The electrostatic interactions between charged beads are described by the Coulombic interaction

$$U_{el}(r) = \frac{q_i q_j}{4\pi\varepsilon_0\varepsilon_r r} \qquad [10]$$

with relative dielectric constant $\varepsilon_r = 20$ in order to include screening. The effect of solvent is incorporated by changing ε_r as well as by varying the degree of dissociation of Nafion side chains. Interactions between chemically bonded beads (in Nafion chains, for example) are modeled by harmonic potentials for the bond length and bond angle

$$V_{bond}(r) = \frac{1}{2}K_{bond}(r - r_0)^2$$
$$V_{angle}(r) = \frac{1}{2}K_{angle}[\cos(\theta) - \cos(\theta_0)]^2 \qquad [11]$$

where the force constants are $K_{bond} = 1250$ kJ/mol.nm and $K_{angle} = 25$ kJ/mol.radian^2 respectively. r_0 and θ_0 are the equilibrium bond length and angle. The size of the simulation box can vary from 50 × 50 × 50 nm^3 to 500 × 500 × 500 nm^3, depending on the system and the composition. We conducted an annealing procedure over a period of 50 ps by increasing the temperature from 298 to 398 K, followed by a short MD simulation for 50 ps in a NVT ensemble, followed by a cooling procedure down to 298 K.[44] We did not observe any drift to a more ordered state after the equilibration procedure. For analysis purposes, however, final trajectories after full equilibration were used.

The degradation process is simulated as the following: first, the initial morphologies are generated using similar set of parameters and

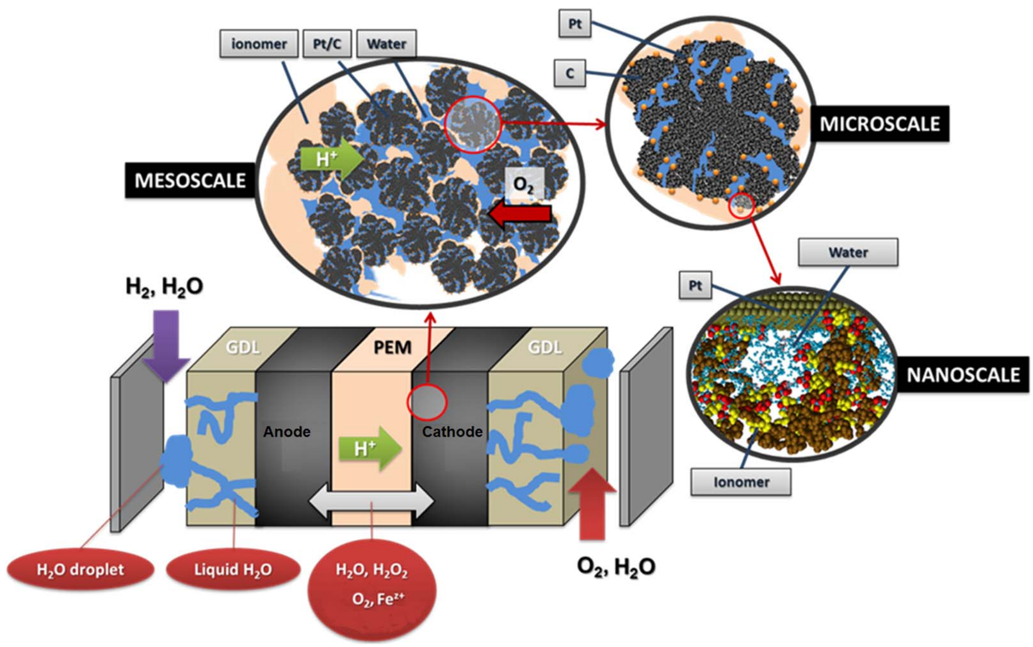

Figure 3. The schematics of the multiscale continuum performance model used in this paper.

process that are explained elsewhere.[44] In order to mimic the degradation process, Nafion sidechains are randomly detached at different percentage from the backbone under various water contents. In our simulations, the detached sidechains are assumed to remain in the water phase inside the Nafion pore as "dissolved" sulfonic anions, thus the system remains electro-neutral.

We have used several tools to calculate structural properties of the degraded membrane to investigate the impact of side chain losses on the microstructural properties of the membrane. These techniques include Radial Distribution Function (RDF), Pore Side Distribution, Cluster Size analysis, and Pore Network Analysis.[43,44,50]

Performance model.—General framework.—The performance model is a multi-paradigm multiscale single-cell model implemented within our in house simulation package MS LIBER-T (see Figure 3).[56–58] This is a software coded in a modular framework on an independent C/Python language basis, highly flexible and portable with multiple application domains already demonstrated.[59,60] Similar to the previous models developed by Franco et al., the single-cell PEMFC model in MS LIBER-T represents explicitly the physical mechanisms at different scales as nonlinear sub-models in interaction (modularity)[61] and it is designed to calculate electrochemical signals (e.g. polarization curves, cell potential vs. time, etc.) from the chemical and structural properties of the materials.[62–65]

For simplicity reasons, in this paper we restrict ourselves on the cell model based on the following overall assumptions:

- isothermal conditions;
- anode operating with water saturated H_2 and cathode operating with water saturated O_2. Under this assumption, the PEM hydration maintains at $\lambda = 19$. From this, only the CGMD database corresponding to this water content is used for the performance decay calculations shown in this paper. We underline that the model is general and other water contents and/or water content transients may be also studied, provided that H_2O transport is resolved across the PEM.

Indeed, the mechanisms described are

- H^+ transport across the membrane electrodes assembly within a 1-D approach;
- e^- transport across the CLs and gas diffusion layers within a 1-D approach;
- the presence of H_2 and O_2 in the on-catalyst ionomer film inside the CLs within the approach reported in Ref. 67. In the case of the anode, a 0D mass balance equation between the O_2 crossover rate from the PEM to the anode and the O_2 consumption rate on the catalyst, is solved to calculate the evolution of the resulting O_2 concentration in the on-catalyst ionomer film (Figure 4b);
- the interfacial nanoscale electrochemical mechanisms at the vicinity of the catalyst including both elementary kinetics and electrochemical double layer effects within an on-the-fly coupled KMC/continuum approach.[66,67] The impact of the surface roughness on the electrochemical double layer structure, as addressed in some publications,[68,69] is not taken into account in the present model.

We use the version of our model which treats the elementary kinetic reactions in the CLs through the Kinetic Monte Carlo Electrochemical Variable Size Method (KMC E-VSSM) that we have introduced and discussed in Ref. 67 for the cathode CL. This approach resolves the adsorption/desorption, adspecies surface diffusion and reactions on the catalyst surface during the PEMFC operation, and allows calculating the electrodes and cell potential.

In general, the performance model can account for the complete cycle of the PEM chemical aging, i.e.: H_2O_2 formation in the anode from the O_2 crossover from the cathode, H_2O_2 formation in the cathode through the ORR, the diffusion of H_2O_2 in the PEM and H_2O_2 decomposition into OH° and OOH° radicals in presence of Fe^{2+}/Fe^{3+} Fenton's cations, the degradation removal of the side chains and the impact on the PEM proton conductivity and cell performance decay (Figure 4).

For demonstration purposes in this paper, the degradation kinetics is assumed to be of first order toward the OH° concentration, i.e.:

$$OH^\circ + R \cdots SC \rightarrow R' + D \qquad [12]$$

where R and R′ refers to the fresh and aged polymer respectively, SC refers to a single side chain and D to the detached side chain. The effect of hydroxide radical in the CGMD simulations is captured by presence of water and hydronium ion and therefore is not explicitly added to the CGMD simulations.

The model implements the CGMD database with spatially resolved 1D resolution across the PEM thickness. The PEM model, comprising the mathematical descriptions of the relevant transport and chemical reaction mechanisms described in the following sections, is coded in Python and coupled as an additional module in MS LIBER-T.

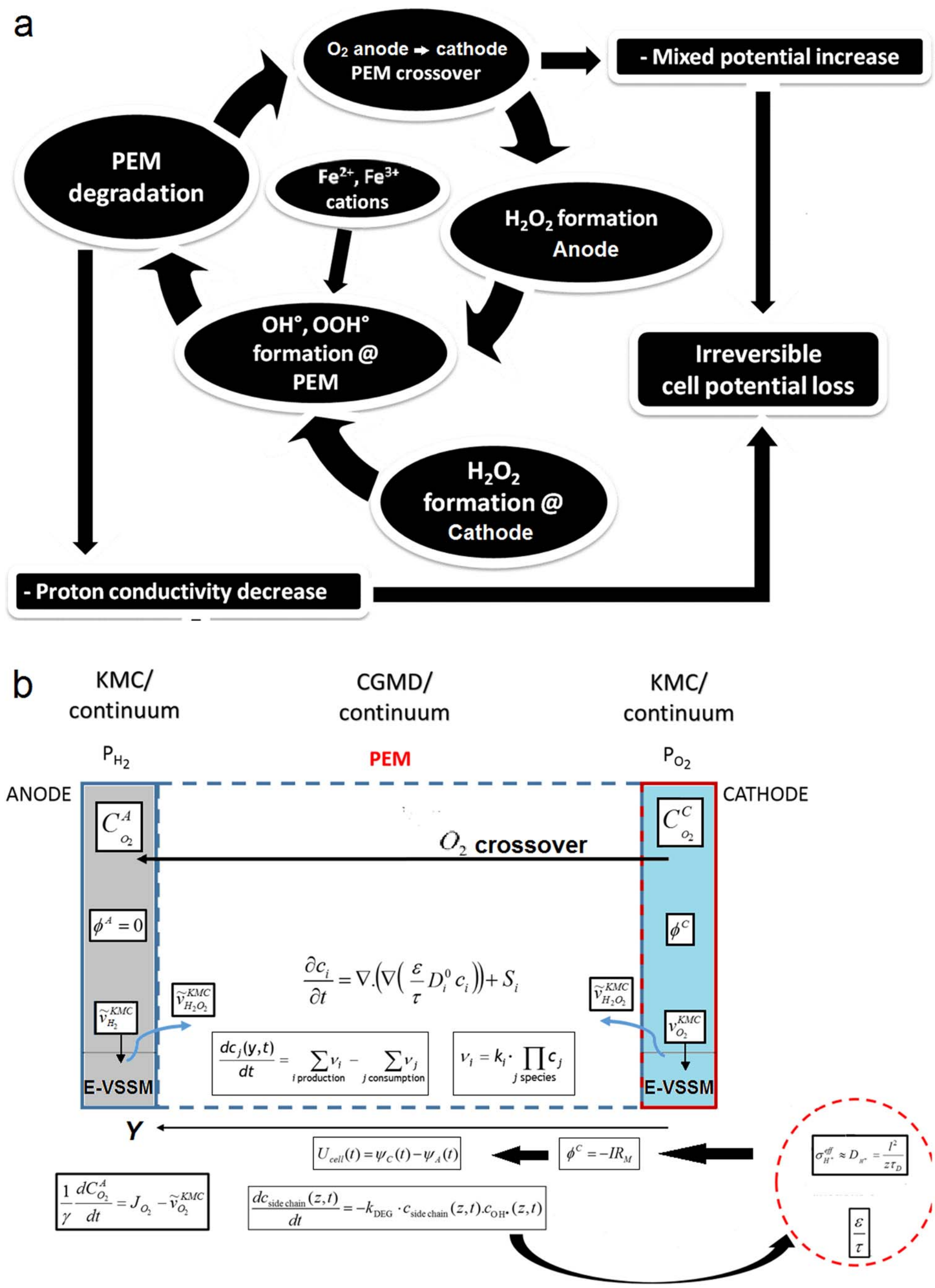

Figure 4. a) Scheme of the complete cycle of PEM chemical aging accounted in our model; b) scheme represented within the cell model.

O_2 transport model in the PEM.—The transport of O_2 is assumed to be simply governed by Fickean diffusion and it is spatially resolved in 1D through the PEM thickness (the H_2 transport was neglected due to its high reactivity at the high potentials typically found in the cathode):

$$\frac{\partial c_i}{\partial t} = \frac{\partial}{\partial y}\left(D_i^{eff}\frac{\partial c_i}{\partial y}\right) \qquad [13]$$

H_2O_2 production models.—The HOR in the anode is modeled in competition with a H_2O_2 production reaction through our KMC E-VSSM approach with DFT-calculated kinetic activation energies. The elementary reaction steps considered are detailed in Table I.[62] Parameter values of the associated electrochemical double layer sub-model and of the surface diffusion processes are identical to the ones used in our previous work.[67]

For the H_2O_2 production within the ORR pathway in the cathode CL, we have considered the elementary kinetic reaction in Table II, still within our KMC E-VSSM approach, with the same parameters values for the activation barriers, diffusion barriers and electrochemical double layer sub-model that in Ref. 67. The reaction steps and the activation barriers values were determined by DFT calculations carried out on Pt(111) surfaces.[62,70] The modular character of the model allows considering here other DFT databases, with different H_2O_2 production rates, corresponding to Pt bimetallic catalysts. This will be the subject of a future publication.

For the adsorption steps we follow the same approach as in our previous publication:[67] according to the collision theory, the kinetic

Table I. Elementary kinetic model for the H_2O_2 production in the anode CL.

Reaction	Activation energies ($kJ.mol^{-1}$) $E_{act}{}^{f}$	$E_{act}{}^{b}$
$H_2 + 2s \underset{k_1/k_{-1}}{\longleftrightarrow} 2H_{ads}$	68	∞
$H_2 + s \underset{k_2/k_{-2}}{\longleftrightarrow} H_{ads} + H^+ + e^-$	34	34
$H_{ads} \underset{k_3/k_{-3}}{\longleftrightarrow} s + H^+ + e^-$	53	53
$O_2^{cross\text{-}over} + s \underset{k_4/k_{-4}}{\longleftrightarrow} O_{2\,ads}$	—	∞
$O_{2ads} + H_{ads} \underset{k_5/k_{-5}}{\longleftrightarrow} HO_{2ads} + s$	41	39
$HO_{2\,ads} + H_{ads} \underset{k_6/k_{-6}}{\longleftrightarrow} H_2O_{2ads} + s$	35	68
$H_2O_{2\,ads} \underset{k_7/k_{-7}}{\longleftrightarrow} H_2O_2 + s$	19	∞

parameters are given by

$$k_i = \frac{sc}{n_{\max}} \frac{P}{\sqrt{2\pi m k_B T}} \qquad [14]$$

where P and m are the partial pressure at x = L (that can be related to the concentration of the dissolved reactant in the electrolyte) and the atomic mass of a reactant respectively. *sc* is the sticking coefficient estimated from published values.[71,72] For the reaction steps, according to the extended transition state theory, the kinetic parameters are given by

$$k_{ij} = \kappa_{ij} \exp\left(-\frac{E^*_{ij,act}}{k_B T}\right) \qquad [15]$$

where k_{ij} and $E_{ij,act}$ are the kinetic rate constant and activation energy along the minimal energy path for going from state *i* to state *j*. The activation energies $E_{ij,act}$ are written as

$$E_{ij,act} = E_{ij,act}{}^{DFT} + f(\sigma) \qquad [16]$$

In Equation 16, $f(\sigma)$ is the effect of the interfacial electric field, function of the catalyst charge density σ, onto the effective kinetics.[62] This quantity together with the concentration of protons in the electrolyte at the vicinity of the reaction sites, is calculated by means of our non-equilibrium electrochemical double layer model in our work.[66]

The KMC E-VSSM allows then the calculation of the evolution of the adspecies coverage on the anode and cathode catalyst surfaces.

H_2O_2 and iron ions reaction-transport models.—The transport of H_2O_2 and iron ions is assumed to be diffusive and they are spatially resolved in 1D through the PEM thickness from the solution of

$$\frac{\partial c_i}{\partial t} = \frac{\partial}{\partial y}\left(D_i^{eff} \frac{\partial c_i}{\partial y}\right) + S_i(y) \qquad [17]$$

where the source/sink term is related to the Fenton reactions describing the H_2O_2 decomposition in OH°/OOH° in presence of the Fenton's cations. In this paper, for demonstration purposes, only the presence of Fe^{2+} and the Fenton reactions reported in Table III were considered.

The concentration of the reaction intermediates, reactants and products are calculated from the mass balances:

$$\frac{dc_j(y,t)}{dt} = \sum_{i\,production} \nu_i - \sum_{j\,consumption} \nu_j \qquad [18]$$

Membrane chemical aging model.—The side chain concentration is resolved from the following balance equation:

$$\frac{dc_{\text{side chain}}(y,t)}{dt} = -k_{DEG} \cdot c_{\text{side chain}}(y,t).C_{OH^\circ}(y,t) \qquad [19]$$

The bulk electrolyte potential at the cathode is given by

$$\phi^{bulk}_{cathode} = -I \times R_{eq} = -\frac{I}{L_{\text{membrane}}} \cdot \int_{y=0}^{y=L_{\text{membrane}}} \frac{dy}{\sigma^{eff}_{H^+}(y,t)} \qquad [20]$$

where $\sigma^{eff}_{H^+}(y,t)$ is the effective proton conductivity calculated from the CGMD database following Equation 6.

Some of the parameters values used are reported in Table IV. The values of the parameters not reported here are the same as in our previous publications.[62]

Table II. Elementary kinetic model for the H_2O_2 production in the cathode CL.

Reaction	Activation energies ($kJ.mol^{-1}$) $E_{act}{}^{f}$	$E_{act}{}^{b}$
$O_2 + s \underset{k_1/k_{-1}}{\longleftrightarrow} O_{2ads}$	—	∞
$O_{2ads} + s \underset{k_2/k_{-2}}{\longleftrightarrow} 2\,O_{ads}$	30	149
$H^+ + e^- + O_{2ads} \underset{k_3/k_{-3}}{\longleftrightarrow} HO_{2ads}$	38	43
$2OH_{ads} \underset{k_4/k_{-4}}{\longleftrightarrow} H_2O_{ads} + O_{ads}$	1	158
$H^+ + e^- + O_{ads} \underset{k_5/k_{-5}}{\longleftrightarrow} OH_{ads} + s$	88	94
$H^+ + e^- + OH_{ads} \underset{k_6/k_{-6}}{\longleftrightarrow} H_2O_{ads} + s$	19	80
$H^+ + e^- + HO_{2\,ads} \underset{k_7/k_{-7}}{\longleftrightarrow} H_2O_{2ads}$	24	47
$H_2O_{2\,ads} \underset{k_8/k_{-8}}{\longleftrightarrow} H_2O_2 + s$	—	∞

Table III. Elementary kinetic model for the Fenton's reactions. The kinetic parameter values are from Ref. 34.

Reaction	Kinetic rate	Kinetic parameter (s^{-1}) k_i
$H_2O_2 + Fe^{2+} + H^+ \xrightarrow{k_1} Fe^{3+} + OH^\circ + H_2O$	$v_1 = k_1 C_{H_2O_2} C_{Fe^{2+}} C_{H^+}$	63.10^{-3}
$OH^\circ + Fe^{2+} + H^+ \xrightarrow{k_2} Fe^{3+} + H_2O$	$v_2 = k_2 C_{OH^\circ} C_{Fe^{2+}} C_{H^+}$	$3.3.10^5$

Results

Membrane meso/microstructure.— PEM simulations were performed with λ = 2, 4, 9, 15. The mesoscopic structure of the hydrated membrane at λ = 9 is visualized in Figure 5, revealing a sponge-like structure, similar to structures obtained by other mesoscale simulations.[75,73] Water beads together with hydrophilic beads of sidechains form clusters, which are embedded in the hydrophobic phase of the backbones. The detailed structural analysis indicates that the hydrophilic subphase is composed of a three dimensional

Table IV. Parameters and numerical values.

Parameter	Numerical value (units)	Source
Temperature (T)	353 K	assumed
k_{DEG}	100	Ref. 35
$S_{electrode}$	2.5×10^{-5} m^2	Ref. 8
Fe^{2+}flux	2.7×10^{-10} $kmol/sec.m^3$	assumed
γ (Figure 4b)	10^{-5}	assumed
$D^{eff}_{H^+}$	1×10^{-9} m/sec	assumed
$D^{eff}_{O_2}$	4×10^{-8} m/sec	assumed
Membrane thickness	2.5×10^{-5} m	assumed
$\sigma^{eff}_{H^+}$(BOL)	2×10^{-4} S/m	assumed
λ	15	assumed

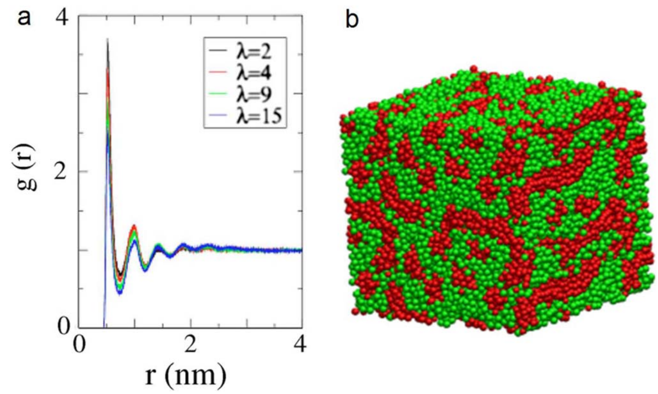

Figure 5. a) RDF elucidating the microphase separation of hydrophilic and hydrophobic domains in Nafion ionomer for side-chain and water;[44] b) a snapshot of the final microstructure in hydrated Nafion ionomer at $\lambda = 9$, obtained from CGMD simulations and before detachment of sidechains. The hydrophilic domain (water, hydronium, Nafion sidechain) is shown in green and hydrophobic domain (Nafion backbone) is shown in red.

network of irregular channels. The typical channel sizes are from 1 nm, 2 nm, and 4 nm at $\lambda = 2, 4, 9, 15$. This corresponds roughly to linear microscopic swelling. The site-site radial distribution function (RDF), obtained from CGMD simulations, matches very well to those from the atomistic MD simulations.[43] The RDF between the sidechain beads and the other components of the mixture show that side chains are surrounded with water and hydrated protons. The autocorrelation functions exhibit similar dependences on bead separation at all $\boldsymbol{\lambda}$, indicating a strong clustering of sidechains due to the aggregation and folding of polymer backbones.[74] The degree of ordering of water near polymer|water interfaces decreases with increasing $\boldsymbol{\lambda}$.

So far, coarse-grained approaches offer the most viable route to the molecular modeling of self-organization phenomena in hydrated ionomer membranes.

Admittedly, the coarse-grained treatment implies simplifications in structural representation and in interactions, which can be systematically improved with advanced force-matching procedures. Moreover, it allows simulating systems with sufficient size and sufficient statistical sampling. Structural correlations, thermodynamic properties, and transport parameters, can be studied.

Figure 6 illustrates tortuosity factor as a function of the sidechain loss (%). Tortuosity factor is defined as a ratio of the geometrical pore length and pore axis. The insert depicts average pore size in nm as function of the degradation at different water contentment ($\lambda = 2, 4, 9, 15$). The diameters of water channels vary in the range of 1–7 nm, exhibiting a roughly linear increase from low to high water content. The average separation of side chains increases as well with water content, which indicates a continuous structural reorganization of polymer aggregates upon water uptake.[44] This could involve backbones sliding along each other in order to adopt more stretched conformations. The sidechain separation varies in a range of 1nm or slightly above. The network of aqueous domains exhibits a percolation threshold at a volume fraction of ∼10%, which is in line with the value determined from conductivity studies. This value is similar to the theoretical percolation threshold for bond percolation on an fcc lattice. It indicates a highly interconnected network of water nanochannels.

In Figure 7a we can see the side chain separation (nm) as a function of the degree of side chain degradation (%) and water content (λ). Overall, by increasing the hydration level, side chains move apart, with their mean separation at Beginning Of Life (BOL) increasing from 0.92 nm at $\lambda = 2$ to 1.48 nm for $\lambda = 15$. Figure 7a also shows that by increasing degradation (percentage of side chains detached from backbone), side chain separation decreases. Side chain separations on a single ionomer chain are between 1.5–1.7 nm.[75] Charge distribution and the magnitude of electrostatic interactions between side

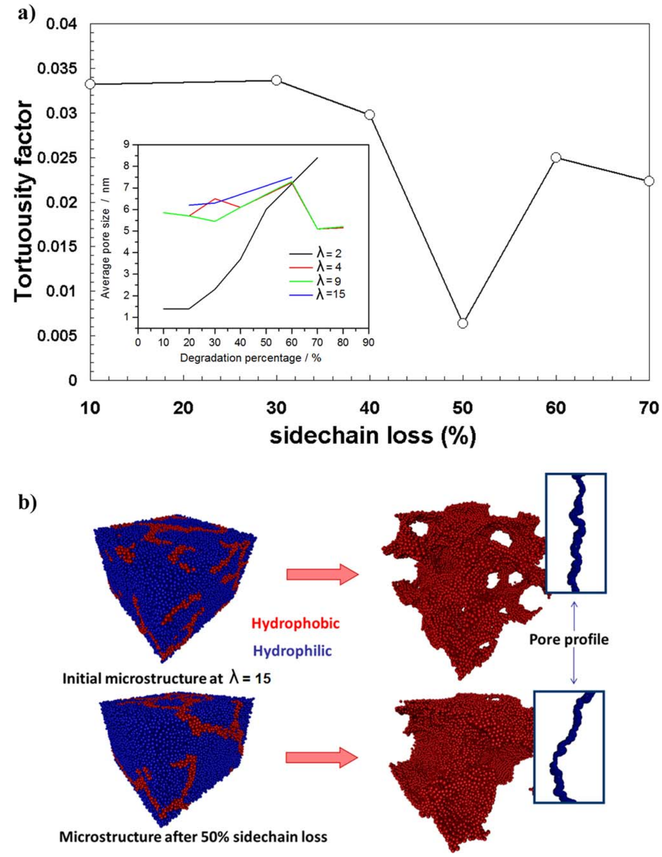

Figure 6. a) CGMD data analysis: tortuosity factor as a function of the sidechain loss (%). Small frame: average pore size in nm as function of the degradation percentage for different water contents ($\lambda = 2, 4, 9$ and 15); b) snapshots of calculated PEM mesostructures for two water contents.

chains determine how ionomer backbones are assembled into fibrils or lamellae, where, the net density of side chains increases. Loss of sidechains reduces electrostatic hindrances between side chains on the surface of fibrils. The latter facilitates easier backbone folding, leading to lower side chain separations. Thus, the effective packing density of side chains due to better polymer degradation indicates that side separations and aggregate sizes decreases with side chain loss. We speculate that decrease in sizes of backbone aggregates corresponds to a decrease in electrostatic interaction between remaining side chains attached to the backbone, which causes increases in packing density of backbones,

In Figure 7b we illustrate normalized average of sidechain separation (d_{ss}) for $\lambda = 9$ with respect to that for the Beginning of Life (BOL) membrane model where no sidechain losses are imposed (%deg = 0). Using a random-walk model for proton diffusion based on the Einstein-Smoluchowski equation[39,76] one can estimate the relationship between proton conductivity, proton diffusivity and mean step distance,

$$\sigma_{H^+}^{eff} \approx D_{H^+} = \frac{l^2}{z\tau_D} \quad [21]$$

where z is a constant dependent upon the dimensionality of random walk (6 for three-dimensional walk), l is the mean step distance, i.e. side chain separations (d_{ss}) and τ_D is the mean time between successive steps. Notice that the above relationship does not necessarily mean protons transfer via a "hopping" Grotthuss mechanism[39] and can similarly describe the *vehicular mass* diffusions. Overall, the normalized relationship between side chain separation and degradation of sidechains depicted in Figure 7b indicates that proton conductivity

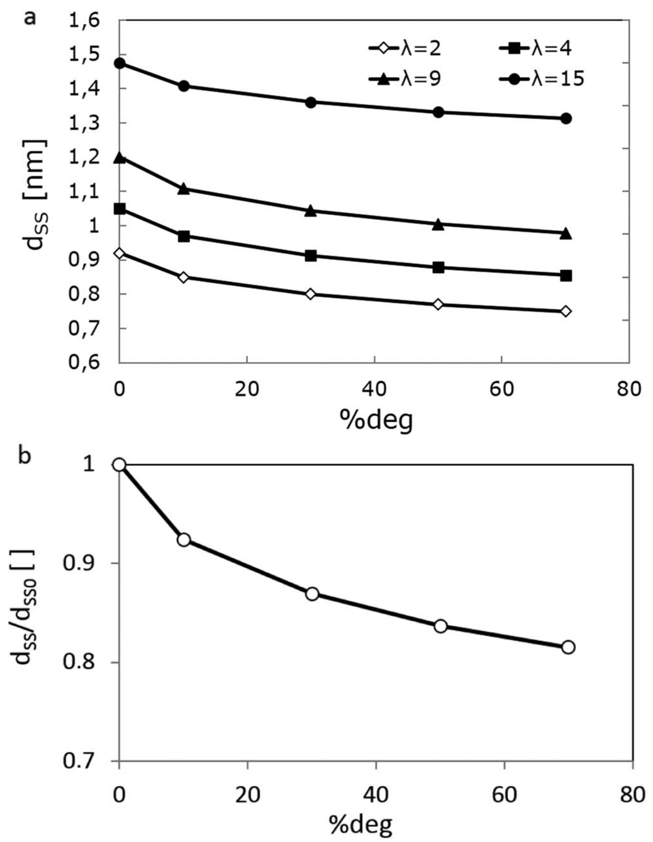

Figure 7. (a) side chain separation (nm) as a function of the degree of side chain degradation (%) and water content (λ). (b) normalized average of sidechain separation (d_{ss}) for $\lambda = 9$ with respect to that for the BOL membrane model where no sidechain losses are imposed (%deg = 0).

is declined by increasing sidechain losses in accordance to the above equation.

Performance decay.— The CGMD-generated database has been used in the performance model following the algorithm presented in Overall methodology section.

We carried out four different simulation cases: OCV, 0.1, 0.3 and 0.5 A/cm^2 applied current densities. For all the cases, the systems were initialized without considering the PEM degradation along the first 0.1 seconds of simulated time, until the steady state is reached: then the degradation process is "activated" by switching on a constant input flux of Fe^{2+} (10^{-14} kmol/m^3.sec). As it is explained in Figure 4, the model allows capturing the HOR and ORR intermediates coverage evolution in both anode and cathode as well as other outputs (such as faradaic current, H_2O_2 production rate, . . .) not shown here. The PEM simulation sub-model calculates the evolution of the porosity/tortuosity, the SO_3^- concentration, conductivity and the associated electrostatic potential evolution across the PEM along the simulation by help of Equation 20.

In Figure 8a, we report the calculated SO_3^- concentration evolution in time for the four cases investigated. The initial SO_3^- concentration was assumed to be 1.2 kmol/m^3 for all the cases. In all the curves in Figure 8a the concentration decays in time with an overall rate which depends on the value of the applied current density. Indeed, the SO_3^- degradation rate increases as the applied current density decreases, which is in agreement with the experimental knowledge. This trend is because of the faradaic current present in the anode, and thus the HOR overall rate (in spite of the H_2O_2 formation), increases with the imposed total current density as the faradaic current evolves to balance it. Briefly, the less H_2O_2 is formed in the anode, the less SO_3^- is degradated.

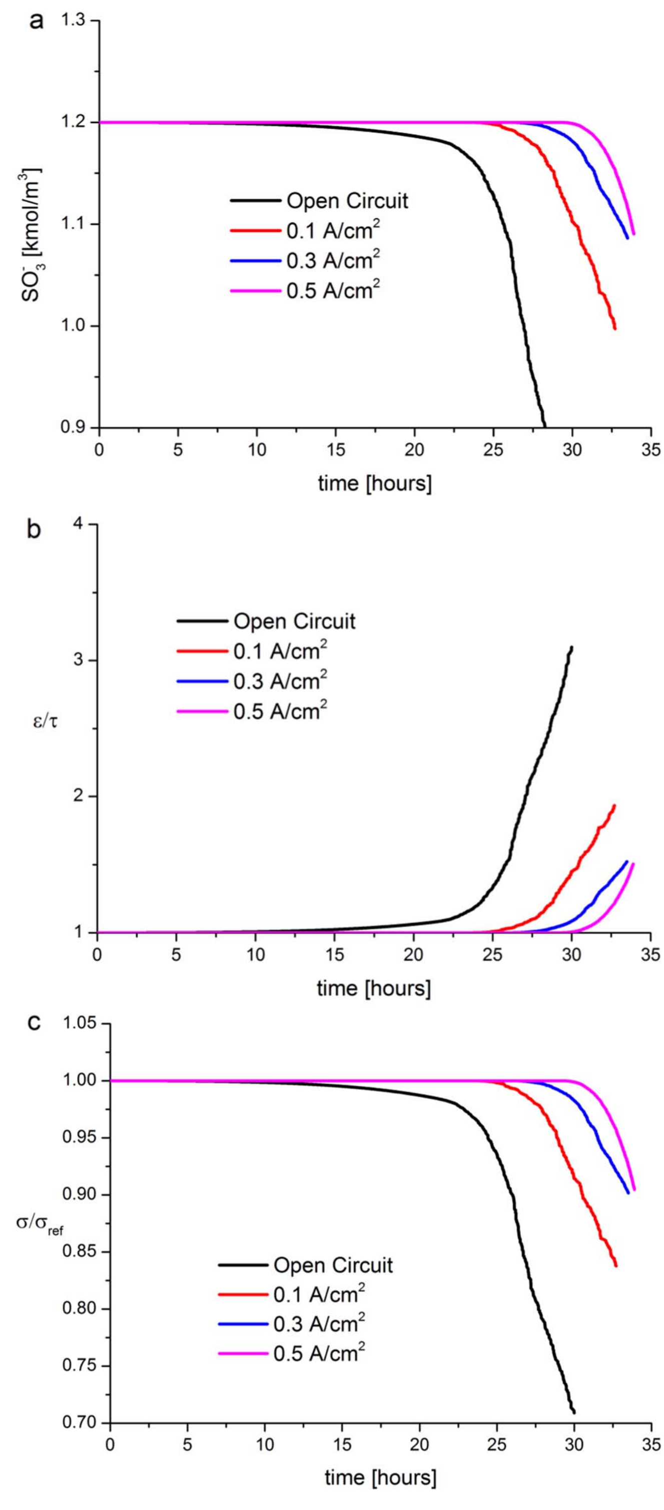

Figure 8. (a) Calculated evolution of the SO_3^- concentration in the PEM at OCV, 0.1, 0.3 and 0.5 A/cm^2 current densities; (b) associated calculated evolution of porosity/tortuosity (normalized in 1 at t = 0 sec.); (c) associated relative conductivity evolution (normalized in 1 at t = 0 sec.).

In Figure 8b we report the corresponding normalized ε/τ evolutions for all the cases under investigation. The SO_3^- consumption generates a decrease on the tortuosity (τ) (see Figure 6) and an increase on the porosity (ε). As one can see, under OCV conditions, this factor varies from 1 to ~3 after 24 hours of simulated time which is in agreement with the experimental known fact that OCV conditions are the most damageable for the PEM.

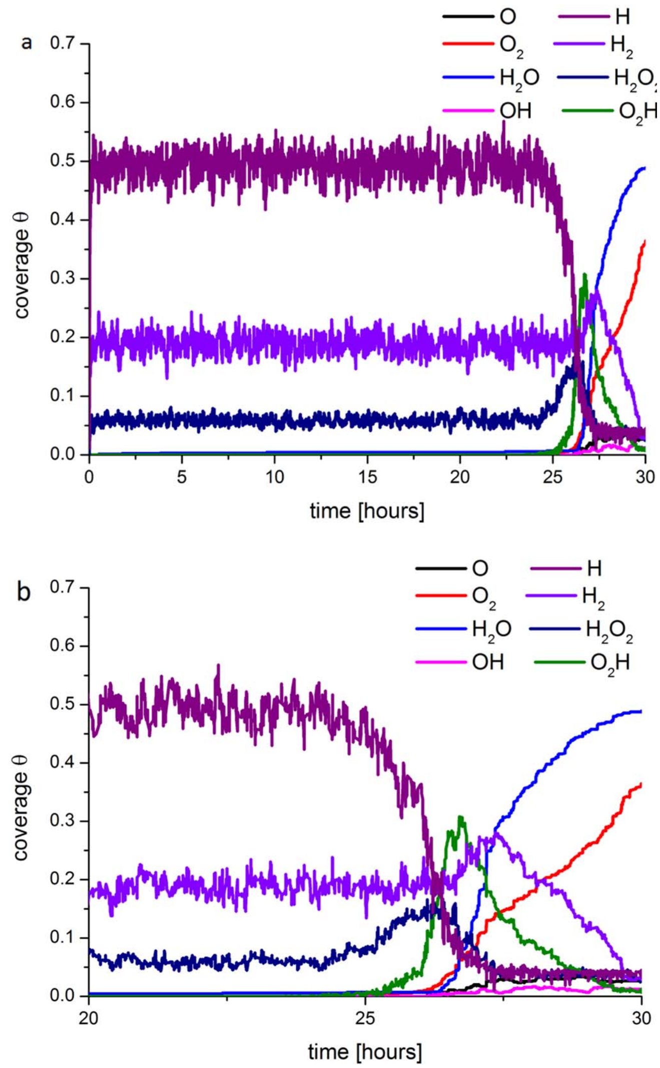

Figure 9. Anode surface coverage evolution under OCV conditions for time intervals between 0 and 30 hours (a) and from 20 to 30 hours (b).

In Figure 8c, the PEM normalized conductivity evolution on time is shown, with a trend which correlates with the increase on the ε/τ factor and the loss of SO_3^-.

We underline that, according to our model, the increase over time of the ε/τ factor during the PEM degradation, leads to a monotonous increase of the effective O_2 diffusion coefficient. The resulting increase of the O_2 crossover leads to the increase of the O_2 adsorption and consequent O formation in the anode catalyst which favors the ORR and the H_2O production. In Figure 9 we present, as an example, the evolution of the adspecies coverage on the anode catalyst under OCV conditions. During the first ∼25 hours of simulated operation, the HOR governs the anode operation with a high coverage of H (∼0.5 ML) and other species such as H_2 (∼0.2 ML) and H_2O_2 (∼0.05 ML). Later, once the O_2 crossover becomes sufficiently high, the anode becomes "cathodized" depleting the overall cell potential. This process is self-maintained because of the retro-feedback with the O_2 crossover: in other words, the more H_2O_2 is produced, the more sidechain loss is induced and finally the more O_2 crossover results, leading again to more H_2O_2 production and so on. Not surprisingly, in Figure 10, we can observe that the PEM degradation does not affect the calculated ORR adspecies coverage for the cathode under OCV conditions.

In Figure 11, we report the cathode ORR coverage evolution for the case of an applied current density of 0.5 A/cm^2. As it was previously predicted[67] the H_2O is the dominant adspecie (with an initial coverage value of ∼0.6 ML for H_2O, 0.3 ML for O_2 and 0.03 ML for O). The PEM degradation process at non-zero current leads to the cathode coverage evolution. Indeed, the cathode responds by increasing the water production as a consequence of the electrostatic potential decrease over time through the PEM (conductivity depletion).

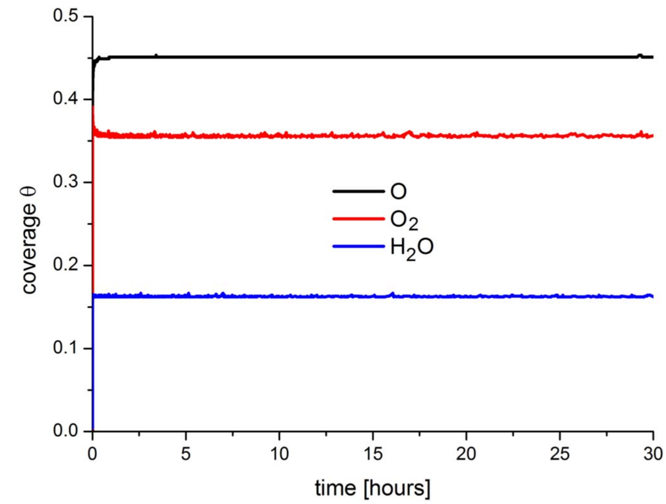

Figure 10. Cathode surface coverage evolution under OCV conditions for a simulated operation time interval between 0 and 30 hours.

In Figure 12, two different simulated time ranges are presented for the HOR coverage evolution in the anode at 0.5 A/cm^2. As one can see around ∼33 hours, the anode starts to generate more H_2O, O_2H and OH, which leads to the cathode potential (the cell potential) decrease over time (Figure 13). This occurs because at ∼33 hours the porosity/tortuosity factor suddenly starts to increase (see Figure 8b), affecting the effective O_2 diffusion coefficient and favoring an undesired ORR in the anode side.

In Figure 13 we summarize the cell potential evolution for the four studied cases. As known from experimental knowledge, under the assumption that PEM aging is the only degradation mechanism involved, the cell performance degradation rate increases as the applied current density decreases. For the three cases where the applied current density is non-zero, the potential decay clearly splits into two regions: first a region until ∼25 hours where the cell potential decays roughly linearly; then a second region where the cell potential decays in a non-linear fashion. According to our model, at non-zero applied

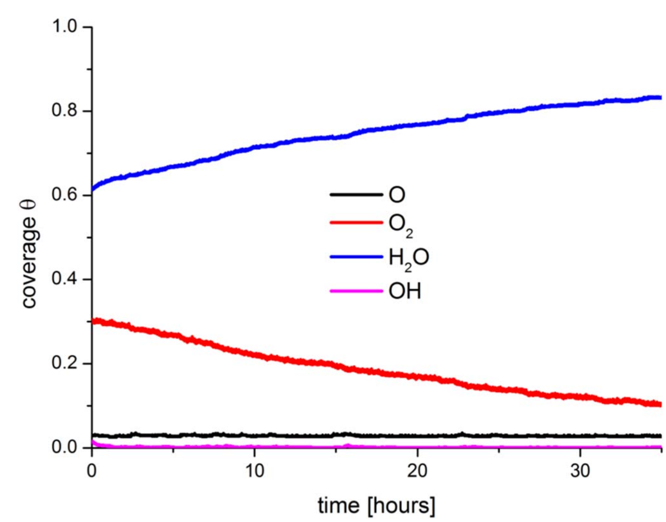

Figure 11. Cathode surface coverage evolution at 0.5 A/cm^2 applied current density for a simulated operation time interval between 0 and 35 hours.

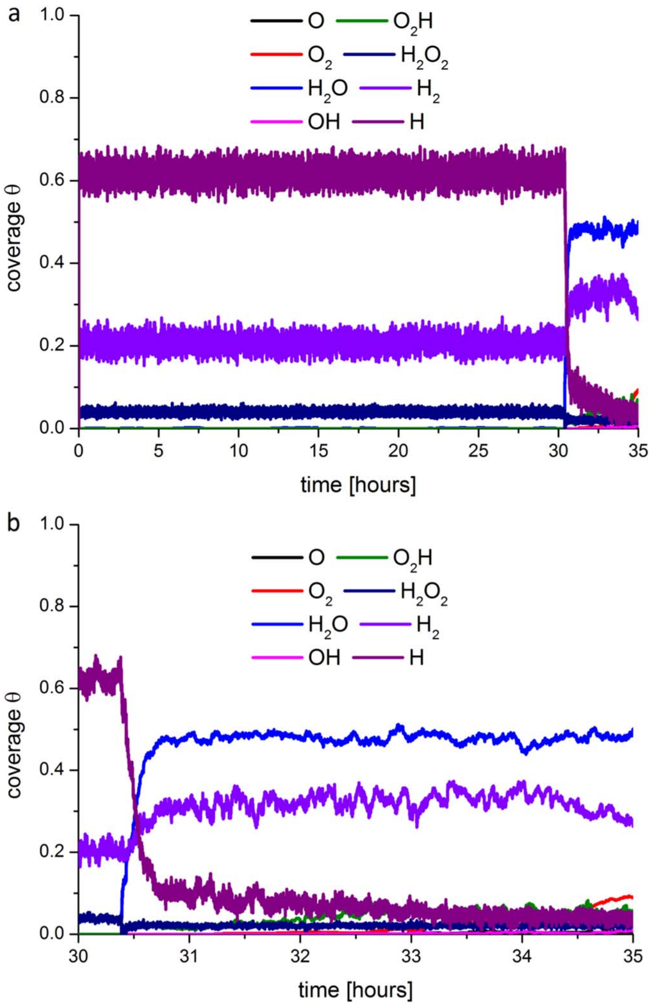

Figure 12. Anode surface coverage evolution at 0.5 A/cm^2 applied current density for simulated operation time intervals between 0 and 35 hours (a) and from 30 to 35 hours (b).

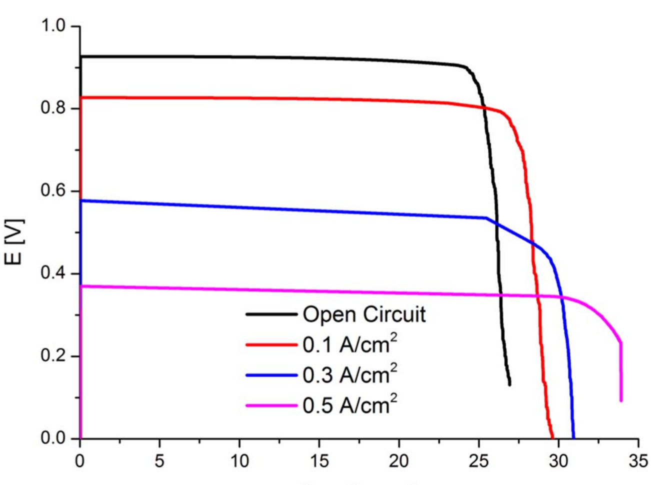

Figure 13. Calculated potential evolution at OCV, 0.1, 0.3 and 0.5 A/cm^2 imposed current densities.

current densities, the first region is governed by the conductivity decrease due to the decrease in the side chain separation (see Figure 7 and Equations 20 and 21); and the cell potential decay in the second region is due to the drastic O_2 crossover increase. At OCV conditions, the overall potential decay is related to the O_2 crossover increase.

Conclusions

In this paper, we have presented a multiscale mesostructurally resolved model allowing predicting the PEM chemically induced aging upon the PEMFC operation conditions. The model is able to simulate both PEM structural changes and performance evolution simultaneously on the basis of a numerical feedback between a performance model and a structural database calculated by CGMD for different aging stages. Calculated trends of the degradation rates and associated performance decays are in good agreement with experimental knowledge.

We believe that this model provides an innovative framework on several aspects:

- the coupling between hybrid KMC/PDE models, describing electrochemistry and transport mechanisms in both anode and cathode, and the (CGMD-based) micro-structurally resolved continuum model describing PEM degradation, proton and oxygen transport. The implementation of the KMC approach allows us to introduce fully atomistically-resolved electrochemical models at the cell level. This provides new capabilities for the simulation of detailed electrochemistry and degradation kinetics in comparison with previous Mean Field/continuum coupled approaches where the lateral interaction and the surface diffusion of adspecies on the catalyst surface cannot be addressed. We underline that degradation processes due to hydrogen peroxide formation strongly depends on the surface diffusion of ORR species in the anode side;
- the CGMD microstructural and degradation database is by itself original, as well as its implementation into the transport/degradation;
- it permits the prediction of the cell durability (i.e. prediction of potential evolution at fixed current) in relation to membrane degradation which is clearly different from previous membrane degradation modeling efforts in literature. In those studies, potential is an input parameter and thus its evolution cannot be calculated independently.

The multiparadigm character of our approach, combining simultaneously CGMD, KMC and continuum modeling, provides insights simultaneously at the atomistic, mesoscopic and macroscopic levels: we are convinced that this provides a powerful tool to the design of more efficient and stable PEMFC materials and/or for the optimization of the operation conditions for enhanced performance and durability.

Incoming work includes the coupling of this multiscale modeling framework with structurally-resolved descriptions of other degradation phenomena (such as carbon corrosion and catalyst degradation) to analyze their competitions, their synergies and their impact on the overall PEMFC performance. Possible future work includes extending this approach to other types of polymers, as well as exploring mechanical degradation aspects.

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References

1. R. Borup, J. Meyers, B. Pivovar, Y.S. Kim, R. Mukundan, N. Garland, D. Myers, M. Wilson, F. Garzon, D. Wood, P. Zelenay, K. More, K. Stroh, T. Zawodzinski,

J. Boncella, J.E. McGrath, M. Inaba, K. Miyatake, M. Hori, K. Ota, Z. Ogumi, S. Miyata, A. Nishikata, Z. Siroma, Y. Uchimoto, K. Yasuda, K.-i. Kimijima, and N. Iwashita, *Chem. Rev.*, **107**, 3904 (2007).
2. A.A. Franco, PEMFC degradation modeling and analysis, book chapter in: *Polymer electrolyte membrane and direct methanol fuel cell technology (PEMFCs and DMFCs) - Volume 1: Fundamentals and performance*, edited by C. Hartnig and C. Roth (publisher: Woodhead, Cambridge, UK) (2012).
3. Polymer Electrolyte Fuel Cells: Science, Applications and Challenges, A.A. Franco, Ed., CRC Press, Taylor and Francis Group, FL, USA (2013).
4. V. Stanic and M. Hoberecht, "Mechanism of pinhole formation in membrane electrode assemblies for PEM fuel cells," *Proc.-Electrochem. Soc.*, **21**, 391 (2004).
5. P. Trogadas and T.G. Fuller, Membrane Degradation Mechanisms in Polymer Electrolyte Fuel Cell, book chapter in: *Polymer Electrolyte Fuel Cells: Science, Applications and Challenges*, A.A. Franco, Ed., CRC Press, USA (2013).
6. S.S. Kocha, J. Deliang Yang, and J.S. Yi, "Characterization of gas crossover and its implications in PEM fuel cells," *AIChE Journal*, **52**, 1916 (2006).
7. M. Danilczuk, F.D. Coms, and S. Schlick, "Visualizing Chemical Reactions and Crossover Processes in a Fuel Cell Inserted in the ESR Resonator: Detection by Spin Trapping of Oxygen Radicals, Nafion-Derived Fragments, and Hydrogen and Deuterium Atoms," *The J. of Phys. Chem. B*, **113**, 8031 (2009).
8. A.C. Fernandes and E.A. Ticianelli, "A performance and degradation study of Nafion 212 membrane for proton exchange membrane fuel cells," *J. of Power Sources*, **193**, 547 (2009).
9. V.O. Mittal, H.R. Kunz, and J.M. Fenton, "Is H_2O_2 Involved in the Membrane Degradation Mechanism in PEMFC?," *Electrochem. and Solid-State Let.*, **9**, A299 (2006).
10. W. Liu and D. Zuckerbrod, "In Situ Detection of Hydrogen Peroxide in PEM Fuel Cells," *J. Electrochem. Soc.*, **152**, A1165 (2005).
11. J. Solla-Gullon, J. Vidal-Iglesias, J.M. Feliu, and A. Aldaz, Electrocatalysis on Shape-Controlled Pt Nanoparticles, book chapter in: *Polymer Electrolyte Fuel Cells: Science, Applications and Challenges*, A.A. Franco, Ed., CRC Press, USA (2013).
12. A.P. Young, J. Stumper, S. Knights, and E. Gyenge, "Ionomer Degradation in Polymer Electrolyte Membrane Fuel Cells," *J. Electrochem. Soc.*, **157**, B425 (2010).
13. H. Tang, S. Peikang, S.P. Jiang, F. Wang, and M. Pan, "A degradation study of Nafion proton exchange membrane of PEM fuel cells," *J. of Power Sources*, **170**, 85 (2007).
14. M. Inaba, T. Kinumoto, M. Kiriake, R. Umebayashi, A. Tasaka, and Z. Ogumi, "Gas crossover and membrane degradation in polymer electrolyte fuel cells," *Electrochim. Acta*, **51**, 5746 (2006).
15. J. Healy, C. Hayden, T. Xie, K. Olson, R. Waldo, M. Brundage, H. Gasteiger, and J. Abbott, "Aspects of the Chemical Degradation of PFSA Ionomers used in PEM Fuel Cells," *Fuel Cells*, **5**, 302 (2005).
16. M. Aoki, H. Uchida, and M. Watanabe, "Decomposition mechanism of perfluorosulfonic acid electrolyte in polymer electrolyte fuel cells," *Electrochem. Commun.*, **8**, 1509 (2006).
17. A. Panchenko, H. Dilger, E. Möller, T. Sixt, and E. Roduner, "In situ EPR investigation of polymer electrolyte membrane degradation in fuel cell applications," *J. of Power Sources*, **127**, 325 (2004).
18. B. Vogel, E. Aleksandrova, S. Mitov, M. Krafft, A. Dreizler, J. Kerres, M. Hein, and E. Roduner, "Observation of Fuel Cell Membrane Degradation by Ex Situ and In Situ Electron Paramagnetic Resonance," *J. Electrochem. Soc.*, **155**, B570 (2008).
19. M.K. Kadirov, A. Bosnjakovic, and S. Schlick, "Membrane-Derived Fluorinated Radicals Detected by Electron Spin Resonance in UV-Irradiated Nafion and Dow Ionomers: Effect of Counterions and H_2O_2," *The J. of Phys. Chem. B*, **109**, 7664 (2005).
20. A. Pozio, R.F. Silva, M. De Francesco, and L. Giorgi, "Nafion degradation in PEFCs from end plate iron contamination," *Electrochim. Acta*, **48**, 1543 (2003).
21. F.N. Büchi, M. Inaba, T.J. Schmidt, J. Scherer, D. Münter, and R. Ströbel, "*Influence of Metallic Bipolar Plates on the Durability of Polymer Electrolyte Fuel Cells, in: Polymer Electrolyte Fuel Cell Durability*", Springer New York, pp. 243 (2009).
22. M.J. Eslamibidgoli, P.-E. Alix Melchy, and M.H. Eikerling, "Modeling the local potential at Pt nanoparticles in polymer electrolyte membranes," *Phys.Chem.Chem.Phys.*, **17**, 9802 (2015).
23. S. Helmly, B. Ohnmacht, P. Gazdzicki, R. Hiesgen, E. Gulzow, and K. A. Friedrich, "Influence of the Distribution of Platinum Deposits on the Properties and Degradation of Platinum-Impregnated Nafion Membranes," *J. Electrochem. Soc.*, **161**(14), F1416 (2014).
24. J. M. Christ, K. C. Neyerlin, R. Richards, and H. N. Dinh, "Concentration Effects of Polymer Electrolyte Membrane Degradation Products on Oxygen Reduction Activity for Three Platinum Catalysts," *J. Electrochem. Soc.*, **161**(14), F1360 (2014).
25. M. Gummalla, V. V. Atrazhev, D. Condit, N. Cipollini, T. Madden, N. Y. Kuzminy, D. Weiss, and S. F. Burlatsky, "Degradation of Polymer-Electrolyte Membranes in Fuel Cells," *J. Electrochem. Soc.*, **157**(11), B1542 (2010).
26. T. Xie and C.A. Hayden, "A kinetic model for the chemical degradation of perfluorinated sulfonic acid ionomers: Weak end groups versus side chain cleavage," *Polymer*, **48**, 5497 (2007).
27. L. Ghassemzadeh, K.D. Kreuer, J. Maier, and K. Muller, "Chemical degradation of Nafion membranes under mimic fuel cell conditions as investigated by solid-state NMR spectroscopy," *J. Phys. Chem. C*, **114**(34), 14635 (2010).
28. D. A. Schiraldi, D. Savant, and C. Zhou, "Chemical Degradation of Membrane Polymer Model Compounds Under Simulated Fuel Cell Conditions," *ECS Transactions*, **33**(1), 883 (2010).
29. T. Ishimoto, R. Nagumo, T. Ogura, T. Ishihara, B. Kim, A. Miyamoto, and M. Koyama, "Chemical Degradation Mechanism of Model Compound, $CF_3(CF_2)_3O(CF_2)_2OCF_2SO_3H$, of PFSA Polymer by Attack of Hydroxyl Radical in PEMFCs," *J. Electrochem. Soc.*, **157**, B1305 (2010).
30. C. Chen and T.F. Fuller, "Modeling of H_2O_2 formation in PEMFCs," *Electrochimica Acta*, **54**, 3984 (2009).
31. L. Gubler, S. M. Dockheer, and W. H. Koppenol, "Radical (HO·, H· and HOO·) Formation and Ionomer Degradation in Polymer Electrolyte Fuel Cells," *J. Electrochem. Soc.*, **158**, B755 (2011).
32. A. A. Shah, T. R. Ralph, and F. C. Walsh, "Modeling and Simulation of the Degradation of Perfluorinated Ion-Exchange Membranes in PEM Fuel Cells," *J. Electrochem. Soc.*, **156**, B465 (2009).
33. K. Kawai, T. Mabuchi, and T. Tokumasu, "Numerical Analysis of Proton Conductivity in Hydrated Nafion Membrane Contaminated with Iron Ion," *ECS Trans.*, **64**(3), 789 (2014).
34. R. Coulon, *Modélisation de la dégradation chimique de membranes dans les piles à combustible à membrane électrolyte polymère*, PhD manuscript, Université Joseph Fourier, Grenoble (2012).
35. R. Coulon, W. Bessler, and A. A. Franco, "Modeling Chemical Degradation of a Polymer Electrolyte Membrane and its Impact on Fuel Cell Performance," *ECS Trans.*, **25**(35), 259 (2010).
36. A. A. Franco, Toward a Bottom-Up Multiscale Modeling Framework for the Transient Analysis of PEM Fuel Cells Operation, book chapter in: *Polymer Electrolyte Fuel Cells: Science, Applications and Challenges*, A. A. Franco, Ed., CRC Press, USA (2013).
37. M. P. Eschenbach, R. Coulon, A. A. Franco, J. Kallo, and W. G. Bessler, "Multi-scale simulation of fuel cells: from the cell to the system," *Solid State Ion.*, **192**(1), 615 (2011).
38. P. Choi, N. H. Jalani, and R. Datta, "Thermodynamics and proton transport in Nafion I. Membrane swelling, sorption, and ion-exchange equilibrium," *J. Electrochem. Soc.*, **152**(3), E84 (2005).
39. P. Choi, N. H. Jalani, and R. Datta, "Thermodynamics and proton transport in Nafion II. Proton diffusion mechanisms and conductivity," *J. Electrochem. Soc.*, **152**(3), E123 (2005).
40. K. H. Wong and E. Kjeang, "Mitigation of Chemical Membrane Degradation in Fuel Cells: Understanding the Effect of Cell Voltage and Iron Ion Redox Cycle," *ChemSusChem.*, **8**, 1072 (2015).
41. K. H. Wong and E. Kjeang, "Macroscopic In-Situ Modeling of Chemical Membrane Degradation in Polymer Electrolyte Fuel Cells," *J. Electrochem. Soc.*, **161**(9), F823 (2014).
42. M. Chandesris, V. Médeau, N. Guillet, S. Chelghoum, D. Thoby, and F. Fouda-Onana, "Membrane degradation in PEM water electrolyzer: Numerical modeling and experimental evidence of the influence of temperature and current density," *Int. J. Hydrog. Energy*, **40**(3), 1353 (2015).
43. K. Malek, T. Mashio, and M. Eikerling, "Microstructure of Catalyst Layers in PEM Fuel Cells Redefined: A Computational Approach," *Electrocatalysis*, **2**, 141 (2011).
44. K. Malek, M. Eikerling, Q. Wang, Z. Liu, S. Otsuka, K. Akizuki, and M. Abe, "Nanophase segregation and water dynamics in hydrated Nafion: molecular modeling and experimental validation," *J. Chem. Phys.*, **129**, 204702 (2008).
45. K. Malek, M. Eikerling, Q. Wang, T. Navessin, and Z. Liu, "Self-organization in Catalyst Layers of Polymer Electrolyte Fuel Cells," *J. Phys. Chem. C.*, **111**(36), 13627 (2007).
46. M. H. Eikerling and K. Malek, "Physical Modeling of Materials for PEFC: A Balancing Act of Water and Complex Morphologies, book chapter in: Polymer Electrolyte Membrane Fuel Cells: Materials, Properties, and Performance", D. Wilkinson Ed., CRC Press, Taylor & Francis 343 (2009).
47. A. Vishnyakov and A. V. Neimark, "Molecular simulation study of Nafion membrane solvation in water and methanol," *J. Phys. Chem. B*, **104**, 4471 (2000).
48. D. A. Mologin, P. G. Khalatur, and A. R. Khokhlov, "Structural Organization of Water-Containing Nafion: A Cellular-Automaton-Based Simulation," *Macromol. Theory Simul.*, **11**(5), 587 (2002).
49. P. G. Khalatur, S. K. Talitskikh, and A. R. Khokhlov, "Structural Organization of Water-Containing Nafion: The Integral Equation Theory," *Macromol. Theory.Simul.*, **11**(5), 566 (2002).
50. K. Malek and A. A. Franco, "Microstructure-based modeling of aging mechanisms in catalyst layers of polymer electrolyte fuel cells," *J. Phys. Chem. B*, **115**(25), 8088 (2011).
51. L. Ghassemzadeh and S. Holdcroft, "Quantifying the Structural Changes of PFSA Ionomer upon Reaction with Hydroxyl Radicals," *J. Am. Chem. Soc.*, **135**, 8181 (2013).
52. D. E. Curtin, R. D. Lousenberg, T. J. Henry, P. C. Tangeman, and M. E. Tisack, "Advanced materials for improved PEMFC performance and life," *J. Power Sources*, **131**, 41 (2004).
53. C. Zhou, M. A. Guerra, Z. M. Qiu, T. A. Zawodzinski, and D. A. Schiraldi, "Chemical durability studies of perfluorinated sulfonic acid polymers and model compounds under mimic fuel cell conditions," *Macromolecules*, **40**, 8695 (2007).
54. S. J. Marrink, A. H. de Vries, and A. E. Mark, "Coarse grained model for semiquantitative lipid simulations," *J. Phys. Chem. B*, **108**(2), 750 (2007).
55. J. T. Wescott, Y. Qi, L. Subramanian, and T. W. Capehart, "Mesoscale simulation of morphology in hydrated perfluorosulfonic acid membranes," *Chem. Phys.*, **12**, 134702 (2006).
56. www.modeling-electrochemistry.com
57. A. A. Franco and K. H. Xue, "Carbon-based electrodes for lithium air batteries: scientific and technological challenges from a modeling perspective," *ECS J. Solid State Sci. Technol.*, **2**(10), M3084 (2013).
58. A. A. Franco, "Multiscale Modeling of Rechargeable Lithium Ion Batteries: Concepts, Methods and Challenges," *R. Soc. Chem. Adv.*, **3**(32), 13027 (2013).
59. K. H. Xue, E. McTurk, L. Johnson, P. G. Bruce, and A. A. Franco, "A comprehensive model for non-aqueous lithium air batteries involving different reaction mechanisms," *J. Electrochem. Soc.*, **162**(4), A614 (2015).

60. K. H. Xue, T. K. Nguyen, and A. A. Franco, "Impact of the cathode microstructure on the discharge performance of lithium air batteries: a multiscale model," *J. Electrochem. Soc.*, **161**(8), E3028 (2014).
61. A. A. Franco, "A physical multi-scale model of the electrochemical dynamics in a polymer electrolyte fuel cell – An infinite dimensional Bond Graph approach"; *PhD Thesis Université Claude Bernard Lyon-1 (France) no. 2005LYO10239* (2005).
62. R. F. de Morais, D. Loffreda, P. Sautet, and A. A. Franco, "A multiscale theoretical methodology for the calculation of electrochemical observables from ab initio data: application to the oxygen reduction reaction in a Pt (111)-based polymer electrolyte membrane fuel cell," *Electrochim. Acta*, **56**(28), 10842 (2011).
63. A. A. Franco, M. Guinard, B. Barthe, and O. Lemaire, "Impact of carbon monoxide on PEFC catalyst carbon support degradation under current-cycled operating conditions," *Electrochim. Acta*, **54** 5267 (2009).
64. A. A. Franco et al. "Pt_xCo_y Catalysts Degradation in PEFC Environments: Mechanistic Insights I. Multiscale Modeling," *J. Electrochem. Soc.*, **156**, B410 (2009).
65. A.A. Franco, *A multiscale modeling framework for the transient analysis of PEM Fuel Cells-From the fundamentals to the engineering practice*, Habilitation (H.D.R.) manuscript, Université Claude Bernard Lyon 1, France (2010). Available online in: http://tel.archives-ouvertes.fr/docs/00/74/09/67/PDF/Alejandro_A_Franco_Manuscript_HDR_July_12_2010.pdf.
66. M. Quiroga, K. H. Xue, T. K. Nguyen, H. Huang, M. Tulodziecki, and A. A. Franco, "A multiscale model of electrochemical double layers in energy conversion and storage," *J. Electrochem. Soc.*, **161**(8), E3302 (2014).
67. M. A. Quiroga and A. A. Franco, "A multi-paradigm computational model of materials electrochemical reactivity for energy conversion and storage," *J. Electrochem. Soc.*, **162**(7), E73 (2015).
68. P. K. Das and S. Bhattacharjee, "Electrostatic double layer force between a sphere and a planar substrate in the presence of previously deposited spherical particles," *Langmuir*, **21**(10), 4755 (2005).
69. P. K. Das and S. Bhattacharjee, "Electrostatic double-layer interaction between spherical particles inside a rough capillary," *J. Colloid Interface Sci.*, **273**(1), 278 (2004).
70. R. Ferreira de Morais, A. A. Franco, P. Sautet, and D. Loffreda, "Interplay between Reaction Mechanism and Hydroxyl Species for Water Formation on Pt (111)," *ACS Catal.*, **5**, 1068 (2014).
71. K. Griffiths and D. Bonnett, "The effects of hidden impurities on the reactivity of a Pt (111) crystal," *Surf. Sci.*, **177**, 169 (1986).
72. D. R. Monroe and R. P. Merrill, "Comparative kinetic studies of CO-O_2 and CO-NO reactions over single crystal and supported rhodium catalysts," *J. Catal.*, **65**, 461 (1980).
73. D. Wu, S. J. Paddison, and J. A. Elliott, "A comparative study of the hydrated morphologies of perfluorosulfonic acid fuel cell membranes with mesoscopic simulations," *Energy & Environmental Science*, **1**(2), 284 (2008).
74. E. Allahyarov and P. L. Taylor, "Role of electrostatic forces in cluster formation in a dry ionomer," *J. Chem. Phys.*, **127**(15), 154901 (2007).
75. K. Malek, M. Eikerling, Q. Wang, Z. Liu, S. Otsuka, K. Akizuki, and M. Abe, "Nanophase segregation and water dynamics in hydrated Nafion: molecular modeling and experimental validation," *J. Chem. Phys.*, **129**, 204702 (2008).
76. J. Philibert, *Atom Movements Diffusion and Mass Transport in Solids*, Les Editions de Physique, Les Ulis (1991).