

Research



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How new concepts become universal scientific approaches: insights from citation network analysis of agent-based complex systems science

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Progress in understanding and managing complex systems comprised of decision-making agents, such as cells, organisms, ecosystems or societies, is—like many scientific endeavours—limited by disciplinary boundaries. These boundaries, however, are moving and can actively be made porous or even disappear. To study this process, I advanced an original bibliometric approach based on network analysis to track and understand the development of the model-based science of agent-based complex systems (ACS). I analysed research citations between the two communities devoted to ACS research, namely agent-based (ABM) and individual-based modelling (IBM). Both terms refer to the same approach, yet the former is preferred in engineering and social sciences, while the latter prevails in natural sciences. This situation provided a unique case study for grasping how a new concept evolves distinctly across scientific domains and how to foster convergence into a universal scientific approach. The present analysis based on novel hetero-citation metrics revealed the historical development of ABM and IBM, confirmed their past disjointedness, and detected their progressive merger. The separation between these synonymous disciplines had silently opposed the free flow of knowledge among ACS practitioners and thereby hindered the transfer of methodological advances and the emergence of general systems theories. A surprisingly small number of key publications sparked the ongoing fusion between ABM and IBM research. Beside reviews raising awareness of broad-spectrum issues, generic protocols for model formulation and boundary-transcending inference strategies were critical means of science integration. Accessible broad-spectrum software similarly contributed to this change. From the modelling viewpoint, the discovery of the unification of ABM and IBM demonstrates that a wide variety of systems substantiate the premise of ACS research that microscale behaviours of agents and system-level dynamics are inseparably bound.

1. Introduction

Literature, tools and methods are important bonds uniting or separating scientific fields. Each research field is built upon the collection, organization and analysis of data on phenomena observed in a very restricted class of systems. This process leads to the formulation of laws and models assumed to respectively govern and describe these systems and serve as the basis for their understanding. As deriving theories are by design each affixed to the discipline from which they stem, the quest for a deeper understanding of the world calls for their extension and validation outside of their original perimeter and, eventually, for their convergence into higher formulations. Transcendence is thus the implicit finality of science, and research integration across disciplinary boundaries the related process, which scientists aim to nurture.

Model-based science [1] provides a good illustration of this need for interdisciplinary research integration. Within this science, disciplines are formed at

the crossroads between modelling paradigms, which each reflect through a specific analytical framework an intrinsic view of systems ontology, and theories, which describe the mechanics of systems studied in a particular research field. Differences in paradigms and emerging theories are of great interest for the advancement of knowledge. At a local scale, the contrasting of models of the same system constructed with different paradigms allows for the observation of diverse facets of its structure and dynamics [2–4]. At the global level on the other hand, confronting a modelling approach to systems encountered in several research fields informs about elements of universality carried by the paradigm itself. Research integration of this second kind may be undertaken in the case of generic mechanistic systems theories spanning over several research fields, as demonstrated henceforth.

The brain, the immune system, ecosystems, societies, financial markets and many other systems are comprised of decision-making agents. Until recently this simple fact has been ignored in virtually all disciplinary theories related to these agent-based complex systems (ACS) [5]. This might be the reason why our understanding and ability to keep these systems within safe operating spaces has been limited [6]. For example, dealing with ecosystems in terms of stocks and flows of nutrients and energy explains many observations but does not capture the role of biodiversity [7], adaptive behaviour [8] and the small population paradigm [9], nor does it acknowledge the holarchic organization visible in nature [4,10]. Likewise, neoclassical economic theories, which assume omniscient, perfectly rational agents, work well under certain circumstances but fail to explain financial crises [11]. The ACS paradigm was born in response to these challenges, yet its study has been undertaken independently in dissimilar fields, resulting in a fragmentation of research under the constraints of disciplinary boundaries.

In the 1990s, with the advent of powerful and cheap computers, the computation of agent-based models (ABMs) became feasible. In these models, system-level behaviours are not imposed but emerge from the behaviour of their agents. Agents and the heterogeneous, dynamic environment, which affects their behaviours and which, in turn, is affected by the actions of agents, are explicitly represented. ABMs are employed whenever one or more of the following aspects are considered essential to understanding system dynamics: adaptive behaviour in which agents make decisions based on their goal, their current state, and the state of their environment; local interactions; and variability in traits of the agents.

Excitement about the potential of this new approach was high, and its ability to unify different theories was hypothesized in 1988 in ecology [12] and approximately a decade later in social sciences [13]. Nowadays, ABMs are employed in all fields dealing with ACS, although their use is new in many. Progress towards general theory has been slow because agent-based modelling has been established independently, along different pathways, in different scientific domains. In ecology among others, ABMs have been referred to as ‘individual-based models’ (IBMs) and initially focused on local interactions and trait variability. By contrast, in social sciences, researchers who employed the term ABM concentrated on adaptive behaviour. Alongside such faint differences in modelling aims between the ABM and IBM communities appeared methodological specificities. For example, the focus on decision-making of humans in sociology led to particular agent-oriented software development methodologies, such as Tropos [14], and design concepts, such as

the belief-desire-intent (BDI) reasoning architecture or more commonly Message Passing [15], which all became central to ABM but are absent of the IBM literature. Depending on constraints, divergences also occurred in specification standards (see §3a, Dynamics of research integration in ACS science), software, and languages used to code models.

Notwithstanding the differences in practices introduced by these parallel evolutions of ACS research, ABM and IBM are inherently indistinguishable from a technical standpoint. They share the same conceptual backbone and fundamental implementation strategy. They both stem from the reductionist idea that system complexity shall be grasped through the study of interactions of fundamental constituents (e.g. crowd or herd behaviour resulting from interdependent individual decisions). Technically, this view is in both cases most frequently implemented in an object-oriented environment inside which the properties and actions of a stereotypic agent (e.g. person, animal, automated system) are algorithmically defined. This inceptive agent then serves as a template to create a population, whose members are left to interact with each other in a virtual world in attempts to mimic empirical observations and infer hidden information about the system studied.

Altogether, the split between ABM and IBM is in essence a matter of terminology and should be terminated, for it may prevent knowledge and methodological progress made in one community to be integrated in the other, and may thereby hinder the emergence of unified systems theories. The exchange of knowledge between the ABM and IBM communities is a necessity to grasp the common essence of systems across sciences and is related to our ability to address fundamental questions, such as whether concepts of social, economical and ecological resilience are related [16]. Methodological progress would also emerge from a fusion of research. For instance, ABM in computer science has benefited from important technological advances, such as high performance computing [17], which could then also profit the IBM community.

The exact dynamics and status of integration of ABM and IBM research have been unclear. To what extent has this purely terminological separation effectively hindered the flow of knowledge in ACS science? Are ABM and IBM further diverging, or, on the contrary, has the presumed potential of agent-based modelling to unify theories across scientific domains been unfolding? Most importantly, in general terms, what factors may foster research integration and lead a concept to overcome disciplinary boundaries and eventually become a universal scientific approach?

I present a method to track quantitatively the integration of scientific concepts across research fields through the analysis of bibliographic citations. This solution was applied to the study of ACS research, which, owing to the artificial terminological separation between ABM and IBM, provided the opportunity to observe how communities may split or merge. To answer the foregoing questions, a bibliometric analysis based on post-processed Scopus records was carried out. The modularity and assortative mixing (i.e. measures of community-based clustering) of publications in the ACS bibliography were assessed, as was the frequency at which publications using the term ABM cited publications featuring the term IBM, and vice versa. The latter analysis was driven by the hypothesis that a possible merger (or, on the contrary, dissociation) of the two modelling communities may be detected through an increase (or decrease, respectively) in overlap of their citation spaces. This

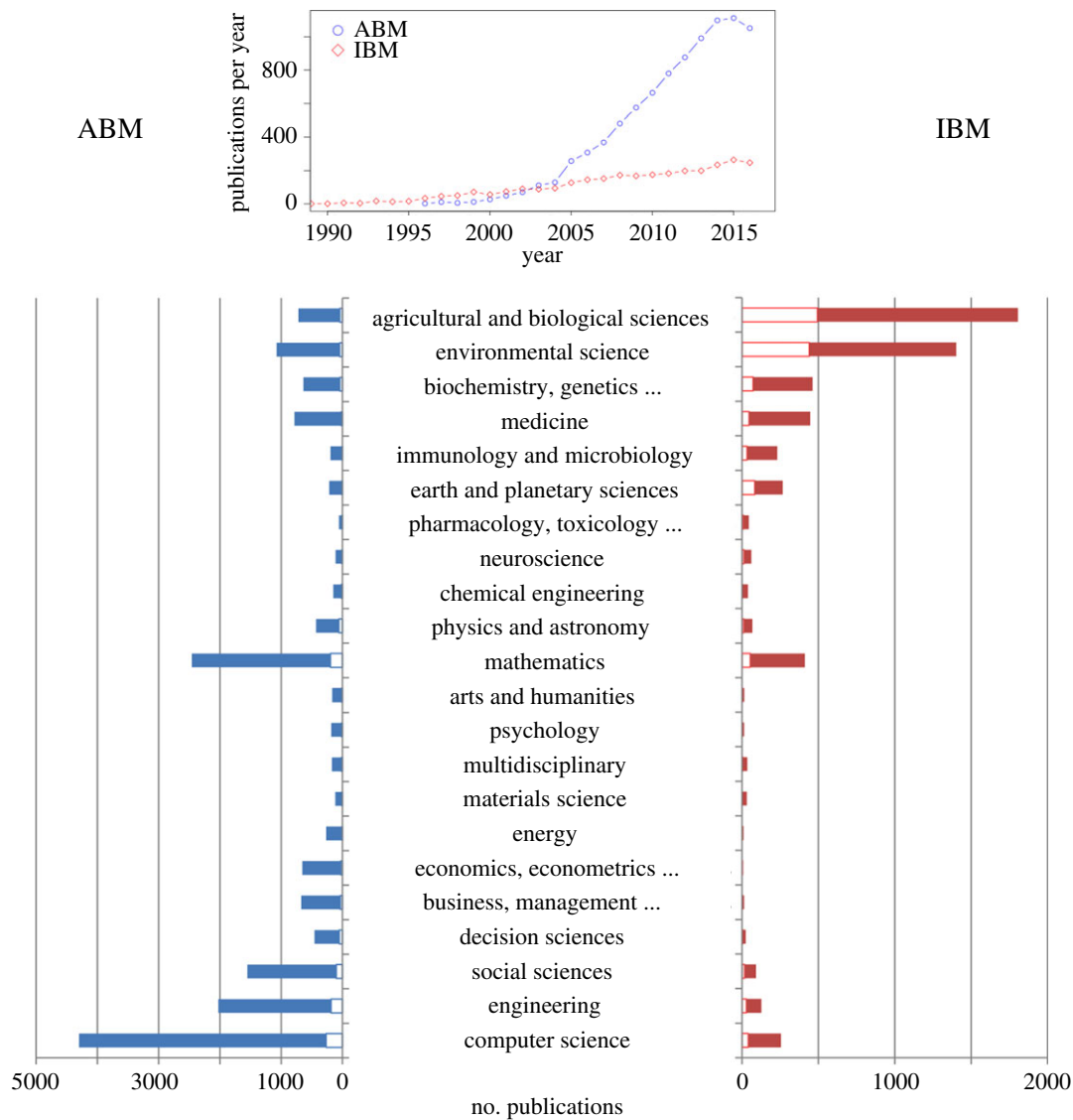


Figure 1. Sciences in which the terms ABM (left) and IBM (right) were dominant until 2005 (empty bars) and post-2005 (solid bars) measured in number of publications referenced on Scopus ($n = 9515$ and 3168 , respectively). Publications can belong to more than one scientific domain. The top inset shows the number of publications per year related to ABM and IBM from 1989 to 2016. Publications belonging to both corpora were counted twice. (Online version in colour.)

method also allowed visualization of the ontology of ACS research and identification of the characteristics of publications that strongly foster science integration.

2. Results

(a) A spread across scientific domains

Between 1990 and 2017, there was a rapid yet asynchronous growth of the IBM and ABM bodies of literature (hereafter referred to as 'corpora') (figure 1, inset). Publications from IBM appeared first, and the numbers grew linearly. ABM scientists first published at the beginning of the new century, and in 2017 ABM had over three times as many publications as IBM. This divergence in growth can be explained by the scientific domains covered by each corpus, which are indicative of a strong specialization. The IBM corpus consists mainly of papers in natural sciences (agriculture, biology, environmental science and medicine), and the ABM corpus focuses on social and formal sciences such as informatics, engineering and mathematics (figure 1). In the last decade, however, a colonization of fields has been taking place (figure 1, empty versus solid bars).

(b) Citation patterns

Only 1.5% of the publications belonged to both ABM and IBM corpora. A comparison with reference corpora representing extreme cases of fully disjointed or synonymous disciplines (comprising respectively 1.5% and 20% of joint publications; see the electronic supplementary material, Extended methodology and figure S1) tends to suggest a clear partition between the ABM and IBM citation networks. This first observation confirms quantitatively a fracture intuitively perceived by seasoned experts.

For further analysis, unweighted directed citation graphs, in which the vertices (or nodes) represent publications and the edges (or links) represent citations, were created automatically for all articles published over certain periods of time. To analyse these graphs, modularity (Q), a metric commonly used to assess community clustering in graphs [18], was employed with a time horizon of one year. This index is based on a comparison between the fraction of edges that fall within given groups and the fraction expected if the edges were distributed at random. A value of Q higher than 0.3 is generally considered as proof of division into clusters [18].

Modularity, which represents here the degree to which the ABM and IBM corpora are isolated from each other, was

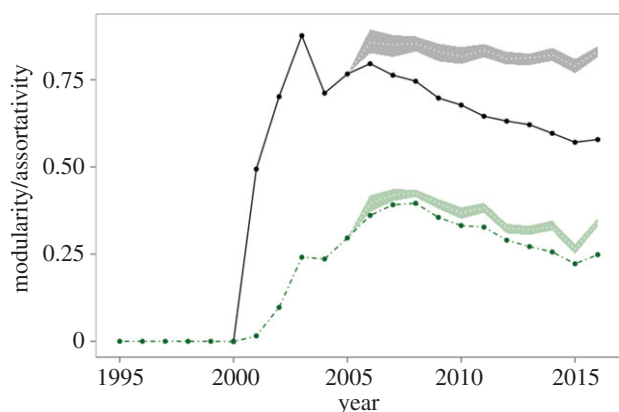


Figure 2. Evolution of community clustering within ACS. Two measures are reported: classic modularity (green dashed line), which describes how clustered the ABM and IBM corpora are, and nominal assortativity (black line), which assesses the level of homophily (i.e. tendency to self-citation) in the two communities. Both metrics were computed annually, i.e. including only papers published in a given year and publications cited therein. Green and black ribbons depict populations of simulated trajectories under the hypothesis of no change in hetero-citation balance from 2005 (see significance of the trend in modularity and assortativity in the electronic supplementary material, Extended methodology). (Online version in colour.)

globally found to have increased sharply during the development of these disciplines (reaching up to a value of 0.4), before decreasing and dropping below the threshold point in recent years (figure 2). Likewise, a significant decline in assortativity and thus in the division between ABM and IBM research was observed beginning in 2005 (figure 2, black line).

Hetero-citation metrics (see Material and methods) further substantiated these results and provided additional insights into the role of each community in the early division and current fusion of the citation network. A lack of mutual awareness between studies using the terms ABM and IBM was unveiled by low proportions of hetero-citations (S_X) and an overall hetero-citation deficiency (D_X) higher than 60% (table 1). Nevertheless, comparing the average hetero-citation in 1988–2004 and 2005–2017 revealed that in the latter period papers included close to three times as many hetero-citations and that the overall hetero-citation balance increased by a third. The annual values of S_X and D_X confirmed that a cross-fertilization had begun around 2006 and that this trend has been steep, constant, and has occurred in both corpora (figure 3). The change was most salient for IBM, which has seen its hetero-citation increase from 0.05 in 2006 to 0.3 in 2017, with a change in heterocitation balance D_X from -91% to -61% . Similar patterns were observed when analysing the hetero-citation of authors instead of publications (see the electronic supplementary material, figure S5).

(c) Dynamics of the fusion

The citation network was visualized using a layout algorithm following which citations, represented as edges, were rendered spatially as attraction forces between publications, represented as vertices (see the electronic supplementary material, Extended methodology). Papers that shared the same references tended thereby to be relatively proximate in the graph and research communities thus clustered visibly.

Tracking the evolution of the citation graph over time shed light on the historical background responsible for the initial division of ACS. In my dataset, individual-based modelling

was first referred to in publications in the late 1980s. This was followed by a clustering process owing to several influential publications: McCauley *et al.* [19], Judson [20] and Uchmanski & Grimm [21] (figure 4a,b). Agent-based modelling, which was first described in the early 2000s, followed a similar process in parallel but with a time lag. The first ABM papers grouped around Parker *et al.* [23] were linked to the IBM corpus (figure 4c). The subsequent clustering of the ABM community occurred around publications including Bonabeau [24] and Macy & Willer [25]. These attractors generated a multipolar community that slowly united while splitting from the IBM counterpart (figure 4d). This fission progressed with the fast growth of ABM literature until about 2005, after which fundamental publications relevant to both ABM and IBM (e.g. Bousquet & LePage [26] and Grimm *et al.* [27]) stimulated fusion of the communities, which remains ongoing (figure 4e).

(d) The role of key methodological papers

A small number of papers had an incommensurate role in sparking the integration process between IBM and ABM. Six ‘fusion papers’ were identified as the main attractors between the two corpora. Three of them were reviews and a book, namely Grimm [28], DeAngelis & Mooij [29] and Railsback & Grimm [30]. The other three publications described methodological advances. Specifically these manuscripts described the ‘ODD’ (Overview, Design concepts and Details) protocol, a standard format for describing IBMs/ABMs (Grimm *et al.* [27,31]), and pattern-oriented modelling (POM), a general strategy for making models structurally realistic (Grimm *et al.* [5]). The publications by Grimm *et al.* from 2006 and 2010 [27,31] were the two most-cited joint ABM-IBM vertices in the graph.

The pivotal role of these six publications was visualized by simply deleting them from the graph and observing the effect on citation network topology (figure 5). Removal of these publications only demonstrated the immediate effects that these papers had in terms of direct citations, and not their indirect contribution (e.g. informing readers about other relevant publications). Still, the consequence of removing them was striking, as it markedly broke the citation network in two separate large clusters, respectively ABM- and IBM-centred.

The great significance of the foregoing papers was confirmed independently by numerical measures of their popularity in both communities jointly using the metric J_i (Materials and methods, equation (4.4); electronic supplementary material, table S1), which is calculated as the minimum between citations counts originating from the ABM and IBM corpora. By contrast, the most referenced paper overall (i.e. Bonabeau [24]) was chiefly cited in the ABM corpus (electronic supplementary material, table S2) and thus had little effect on the fusion process (electronic supplementary material, figure S3). The influence of the six fusion papers was corroborated by their prevalence in the citation chains forming the citation graph, as expressed by betweenness centrality (BC) measures (electronic supplementary material, table S3; see Materials and methods for explanations on BC). Hence, the small set of papers that triggered the fusion became some of the most important references in ACS science.

Software is most often not directly linked with indexed publications. Modelling platforms, which are central to modelling practice, were thus absent from the citation graph but were analysed separately (see the electronic supplementary material, Extended methodology). The reconstruction of J_i metric values for four common ABM/IBM tools demonstrated that some

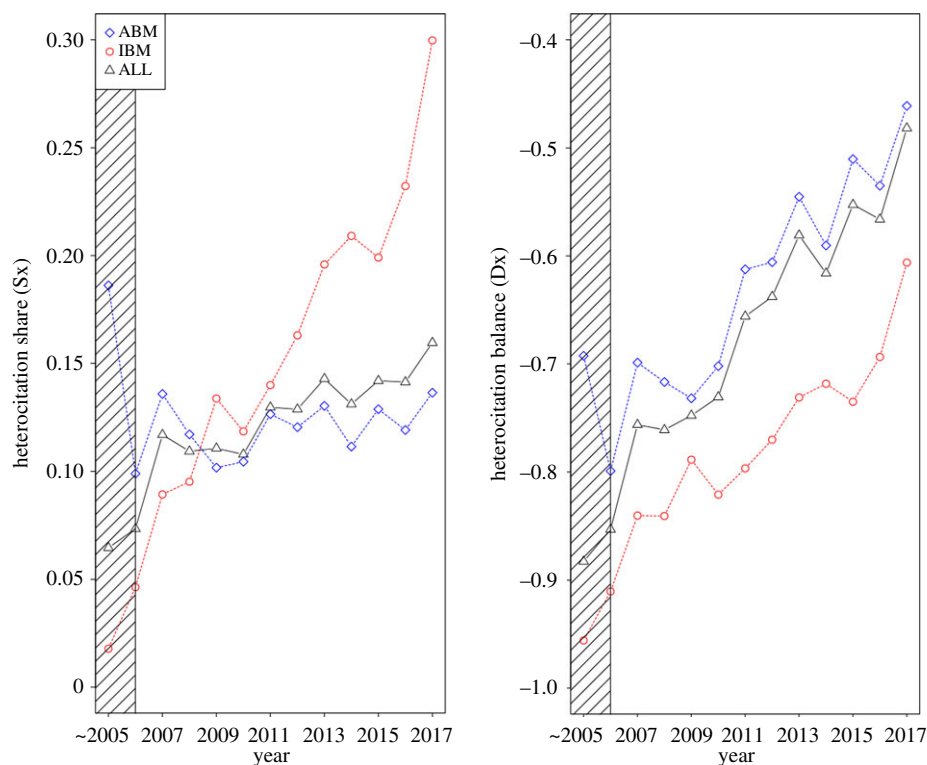


Figure 3. Evolution of the annual hetero-citation share S_x and balance D_x for papers published from 1989 to 2017. Left: time-series of the hetero-citation share for the ABM (blue) and IBM (red) corpora and overall (black). Right: hetero-citation balance, i.e. the relative difference between the observed and expected hetero-citation S_x . Metric values before 2006 (shaded area) were averaged over the past period to obtain significant values. (Online version in colour.)

Table 1. Hetero-citation metrics based on bibliographic references. S_x (in parenthesis) represents the average proportion of citing of publications belonging to the other community; this metric ranges from 0 to 1, corresponding to citation networks where all papers of a community A cite only papers within ($=0$) or outside of A ($=1$), respectively. D_x represents the deviation between the observed S_x and the value expected when taking into account the difference in size between corpora A and B.

D_x : the relative difference with the expected hetero-citation share S_x (in parenthesis, S_x , the vertex-level share of referencing to the other community)						
corpora (A/B)	A		B		overall	
ABM/IBM	1988–2004	2005–2017	1988–2004	2005–2017	1988–2004	2005–2017
	–69% (0.209)	–59% (0.121)	–98% (0.007)	–78% (0.157)	–93% (0.045)	–64% (0.129)
CA/ANN	–89% (0.06)		–98% (0.01)		–95% (0.03)	
RSI/CTD	+13% (0.73)		–14% (0.49)		–2% (0.59)	

pieces of modelling software had a non-negligible impact on the fusion process (electronic supplementary material, figure S4). While Repast's or SWARM's contributions were significant yet modest compared to the publications listed above ($J_i = 8$ and 7 respectively), Netlogo [32] ($J_i = 39$) had an effect comparable to Grimm [28], which ranked fourth among the six key papers. Interestingly, Netlogo has begun to have an impact from 2011, so globally later than the top publications, except Grimm *et al.* [31] with which it shared an apparently synchronized growth pattern.

3. Discussion

(a) Dynamics of research integration in agent-based complex systems science

Graph theory, and more specifically citation network analysis, has proved very useful in the study of the dynamics of scientific

communities. It has, for instance, been recently employed to detect 'sleeping beauties' in science [33], to understand the meaning of terminologies across fields [34], to reveal manuscript submission patterns [35] and to assess the stability of communities [36]. I employed it in the present study to gain insight on mechanisms of science integration.

Research in social network analysis has shown that scientific communications reproduce cognitive structures, and consequently citation patterns are a good proxy for subjacent intellectual organization [37]. Thus, it was presumed here that the interrelatedness of the ABM and IBM communities could be evaluated by determining how intertwined their corpora were, which could be studied bibliometrically. The underlying assumption was that a united scientific discipline would generate a collection of papers that features well-mixed references to publications within the same corpus, without noticeable segregation.

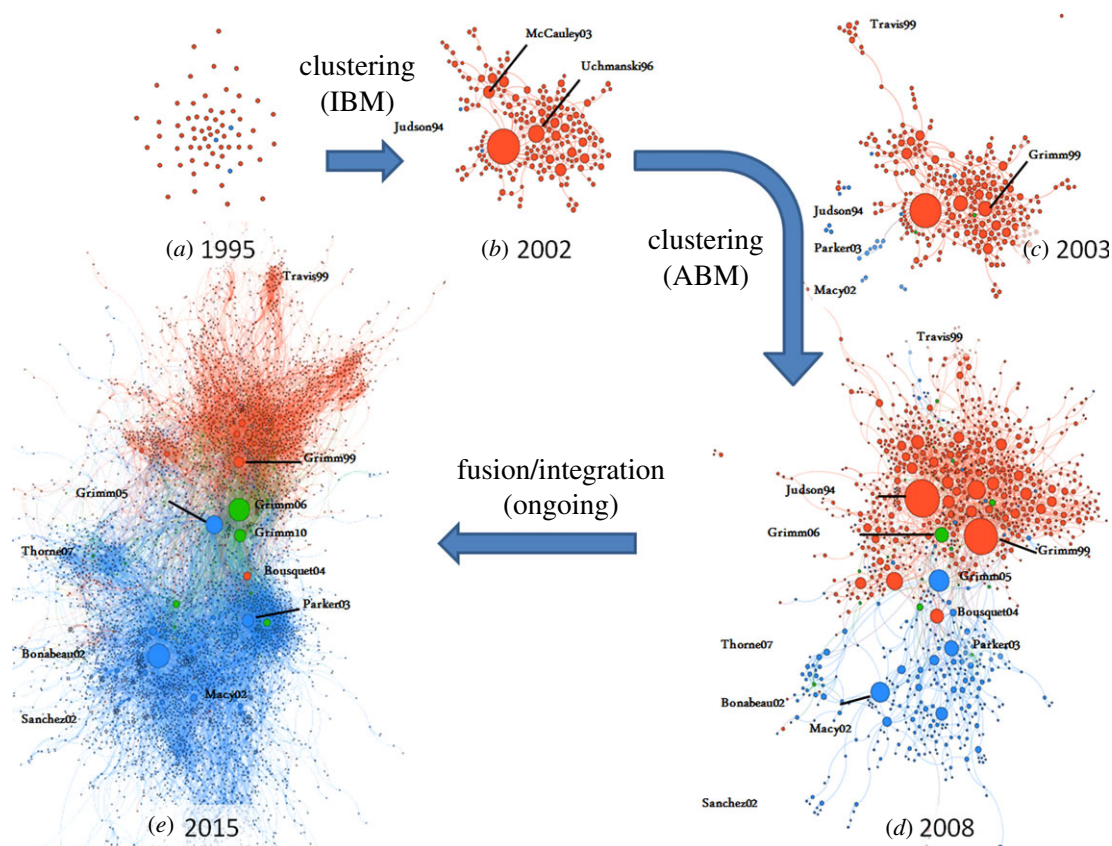


Figure 4. Evolution of the citation graph of ABM/IBM literature over time. Publications are represented by vertices (blue for ABM, red for IBM and green for both), which are attracted to each other proportionally to the number of edges (i.e. citations) linking them. Important publications are labelled with first author name and publication year. For full citations, see references and the electronic supplementary material, table S3. Vertex size is proportional to the number of citations within each time-dependent subgraph, but scaling varies between subgraphs. (a) IBM papers appeared first, but had weak interconnections. (b) A clustering then took place after the appearance of influential papers. (c) ABM papers followed the same pattern with a lag of a decade. (d) Clustering of the ABM corpus occurred around central papers. (e) Fusion of ABM and IBM emerged under the impulse of key papers. The formation of sub-clusters is also visible; for example, publications centred around Thorne *et al.* [22] focused on cell-scale agent-based models. (Online version in colour.)

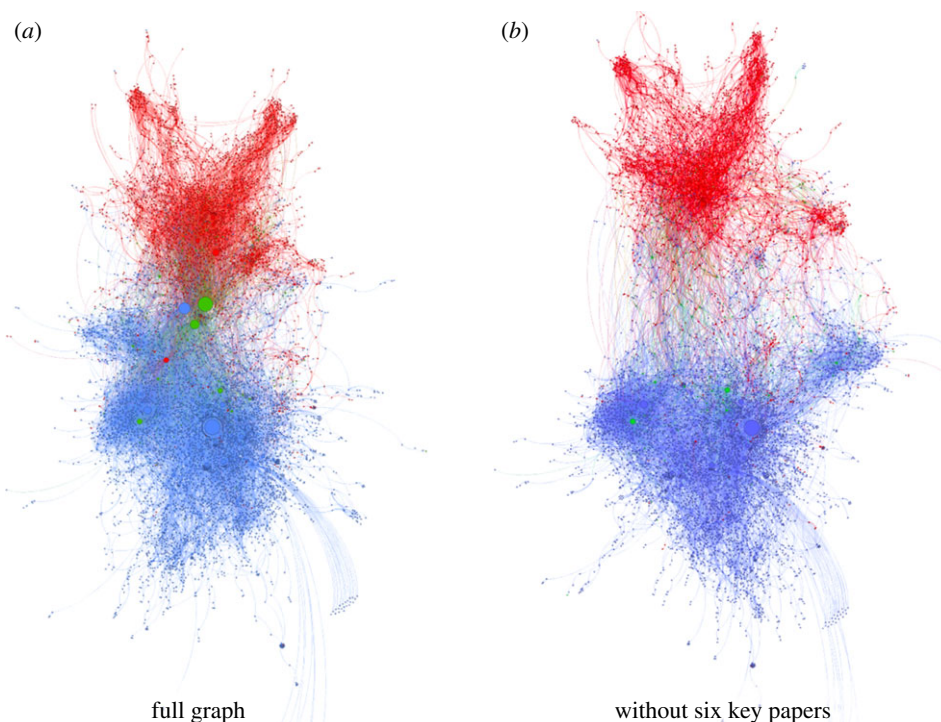


Figure 5. Citation graph of the ACS literature (a) with and (b) without six key publications. Citations act as a cumulative attraction force between papers. The more references publications share, the closer they are located on the graph. (Online version in colour.)

The implicit division of ACS research into two impermeable communities with a focus on the same object of study and compatible methods but different sets of research fields was unnatural, yet this aberrant state lasted for a long time. The analysis described here did not begin with the assumption that the emergence of ACS science was occurring nor were individual publications expected to play a major role in initiating a potential fusion. Nevertheless, a recent ongoing fusion of the communities—albeit barely perceptible to their members—was detected in this study. The fusion was visible as a spread across scientific domains (figure 1, plain bars) as well as through temporal variations in hetero-citation balance (table 1) and network modularity/assortativity (figure 2), which showed a trend toward a merging of the citation networks since 2006. These observations may suggest an ongoing cross-fertilization that is leading to a fusion of the communities. The more frequent recognition in recent years that ABM and IBM shall be considered equivalent [38–41] corroborates this hypothesis. For instance, the latest book by Railsback & Grimm [30] was titled '*Agent-based and individual-based modeling: a practical introduction*', whereas their previous book [42] had mentioned only '*Individual-based modelling and ecology*'.

These results raised two interlinked questions: How did division initially occur? What put an end to it? The first question was answered by retracing the temporal evolution of the bibliographic network (electronic supplementary material, movie S1); this showed that the development of the two communities was generated by an asynchronous integration of ACS research in different fields (figures 1 and 3). To my surprise, the fall of this deep-rooted division was triggered by only a handful of publications (figure 5). The reason why precisely the division of ACS research lasted so long and was ended by a very small number of publications possibly relates to the conditions necessary for transdisciplinary science integration conjectured on in the following.

Tracing the birth of ACS science incidentally represented an opportunity to better understand the creation process of a science (or at a lower level, of a research area, for what is described hereafter appears to be a fractal phenomenon). A pattern consisting of phases of clustering around focal publications—related to research fields—and integration of these clusters into larger communities and ultimately into a united science was revealed by the analysis of the dynamic graph (electronic supplementary material, movie S1; figure 4). These clustering processes can be assumed to be routine in the development of science. The mechanisms driving the final unification between ABM and IBM may be understood by looking at the nature of the few papers that sparked the fusion. In chronological order of appearance, reviews were the first element of the science integration process, and were followed by publications on a standardized protocol and on global methodologies. This observation leads to the hypothesis that at least three conditions are required for a science to emerge: the awareness of joint issues, ways of communication, and transcendental concepts and methods.

The awareness of joint issues is evidently a *sine qua non* condition and the absence thereof is precisely what initially favoured the independent growth of ABM and IBM as these communities were rooted in separate sets of scientific branches (figure 1). Reviews are obvious vectors for awareness raising as their very purpose is to make the current state of knowledge on a topic accessible to readers external to the research field. Successful reviews are thus expected to foster integration.

For a considerable time, a lack of communication prevented the merger of IBM and ABM. Initially, the IBM community had no generic way to describe its models, and the ABM community had developed several incompatible specification languages derived from the study of multi-agent systems (e.g. the Z-notation [15], the Gaia framework [15] and Prometheus [43]). This state promoted the further separation of the ABM and IBM communities. In addition, ABM and IBM researchers published in journals specialized in different fields, generating papers with formalisms that were inaccessible to the other community. This largely explains the delay preceding fusion. Thus, solving this communication issue seems to be the most important step in science integration, as shown here by the outstanding impact of the first ODD methodology paper [27] (electronic supplementary material, tables S1 and S3). Modelling software, and more particularly Netlogo [32], also nurtured the unification by providing a common technical backbone for model implementation as well as meeting venues in the form of online forums and dedicated conferences (e.g. Swarmfest). The simultaneous growth in importance of Netlogo and Grimm *et al.* 2010 [31] from 2011 (electronic supplementary material, figure S4) and the publication on that same year of the reference book by Railsback & Grimm [30], which provided an updated practical introduction to IBM with examples in Netlogo, may suggest that these three works have promoted one another and acted in synergy to stimulate communication among practitioners of ACS research.

The awareness of joint issues and ways of communication are possibly enough to allow interdisciplinary work based on a similar framework, but, ultimately, they are insufficient to give rise to a self-standing science. For this purpose, boundary-transcending concepts and methods are required that provide an autonomous life to an interdisciplinary research field. POM [5,44] was therefore proposed as a general strategy for improving the structural realism of models by requiring reproduction of several observed patterns simultaneously, thereby reducing the risk a model produces the right answers for the wrong reasons. This strategy basically reflects how science proceeds in principle [45] and is independent of the field in which a model is developed.

(b) Future implications of the slow rise of agent-based complex systems science

The idea of a general systems theory is compelling. It holds the promise that general principles exist, which, independent of the idiosyncrasies of the building blocks involved, explain and help predict the structure and dynamics of complex systems. Examples include the theories of general systems [46], cybernetics [47], hierarchy [48], networks [49], and, more recently, complex adaptive systems (CAS; [50]). All these theories capture important aspects of complex systems, but they start from a certain system-level concept and are thus top-down approaches.

A general bottom-up theory of ACS, based on agent-based modelling, could complement these theories by starting from the systems' building blocks: decision-making agents and their interactions. Identifying general principles then requires exploring the emergence of patterns across different levels of organization, scales, entities and systems.

To my knowledge, the mechanisms underlying research integration are poorly understood and little is known about the means at the disposal of scientists to stimulate this process. Moreover, following the general fusion of disciplines,

the conditions under which a science is declared born remain undefined. Despite not offering decisive answers to these open issues, I proposed a method for quantifying the dynamics of a discipline (through assortativity, heterocitation metrics and pattern verification based on bibliographic network analysis), which represents a progress towards these goals. Some hypotheses were proposed in the present paper as to how and under which conditions research integration in disjunct scientific communities rooted in different research fields can take place. These are left to be further verified and generalized, and follow-up works will be necessary to obtain a clear picture of the processes at play. Fortunately, agent-based models could serve as an opportune framework to simulate citation dynamics and provide finer understanding of how human factors influence citation patterns and community formation in science. In addition to enhancing our grasp of the sociology of science, this study provided insights into ways of detecting detrimental situations (such as the unnatural division of ACS research) and guide scientific undertakings to maximize their impact on a given field of study.

This novel approach provided quantitative signs of the self-sustaining emergence of a unified transdisciplinary science of ACS. This important finding tends to indicate that the connectionist and reductionist paradigm on which ACS relies is not only valid in ecology as initially postulated but is inherent to most scientific research fields. It can be reasonably expected that, as cross-disciplinary integration continues under the framework of ACS research, unified theories about how complex system behaviours emerge from interactions between agents will come forth.

4. Material and methods

(a) Data collection and preprocessing

The dataset supporting this study was built upon Scopus records. Non-indexed papers and grey literature were consequently unaccounted for. Two queries were sent on 14 April 2017 to Scopus to construct separately the ABM and IBM corpora by selecting all papers including ‘agent-based model*’ and ‘individual-based model*’, respectively, in title, abstract, or keywords. An R script based on DIDEROT [51], a package specifically designed to support this study, processed the resulting datasets, which were first merged and cleaned of spurious entries and duplicates. Data on 12 504 publications, including 466 346 citations, were obtained. Precise publication dates were retrieved based on digital object identification (DOI) codes using automated queries to the website of the International DOI Foundation.

References were then extracted from each record and used to link publications with one another to produce an unweighted directed citation graph. The latter was pruned of unidentified vertices (i.e. references absent from my dataset). Statistical analysis was performed on the resulting graph (12 504 vertices and 27 476 edges).

(b) Graph modularity, assortative mixing and hetero-citation analysis

Natural network clustering is generally characterized using the concept of modularity, which represents the strength of division of a network into subgraphs of densely connected vertices. The analysis performed here was based on classical modularity as defined by Newman & Girvan [18]. Citation graphs of scientific publications allow for only one edge between two vertices (i.e. references cannot be redundant), and they do not lose edges in

time (i.e. references do not disappear), nor do new edges grow between existing vertices (i.e. new references cannot be added to papers after publication). Therefore, modularity in such graphs tends to persist over time. This inertia results after several years in a very slow rate of change of the modularity coefficient, which does not visibly render recent variations in community clustering (see the electronic supplementary material, figure S2). For this reason, in order to study the development in time of modularity, the domain of application of the formula was limited to the vertex-induced graph including only papers published within the year under scrutiny as well as all papers cited therein, i.e. $Q(\text{year}) = Q(G(\text{year}))$ with:

$$G(\text{year}) = \{V_i \mid \text{Year}(V_i) = \text{year} \vee (\text{Year}(V_k) = \text{year} \wedge \exists E_{V_k \rightarrow V_i})\}, \quad (4.1)$$

where $E_{V_k \rightarrow V_i}$ represents an edge from vertex V_k to V_i .

The modularity score was complemented by the assortativity coefficient r assessing the level of mixing by discrete vertex characteristics [52] (here, corpus association) over the same time-restricted graphs. This normalized metric, which basically renders the ratio between observed and theoretical maximum modularity of a given graph, is insensitive to changes in corpora sizes and evaluates the tendency of communities to cite themselves (so-called homophily in social networks). The significance of the trends observed in both scores was assessed through parametric bootstrapping (see the electronic supplementary material, Extended methodology).

The foregoing two metrics were, however, not exhaustive. As parameter-free data mining techniques, conventional modularity-derived metrics were mainly designed to detect concealed communities. They are thus generally suboptimal when used to inform on patterns of awareness between pre-identified communities in asymmetrical cases (e.g. corpus A cites frequently corpus B, but not the other way around). For this reason, a finer measure of connectivity of a corpus X in relation to a corpus Y , which is referred to here as hetero-citation share S_X , was additionally advanced:

$$S(V_i) = \frac{N_Y(V_i)}{N_{X \cup Y}(V_i)} \quad \text{and} \quad S_X = \frac{1}{n_{X^*}} \sum_{V_i \in X^*} S(V_i) \quad (4.2)$$

where $\begin{cases} N_Z(V_i) : \text{number of citations from } V_i \text{ to a given corpus } Z, \\ X^* : \text{corpus } X \text{ without leaf vertices or vertices belonging} \\ \text{also to } Y, \\ n_Z : \text{number of vertices in a given corpus } Z, \\ \text{i.e. } \#E_{V_i \rightarrow V_k, V_k \in Z} \\ \text{i.e. } \{V_i \in X \setminus Y \mid N_{X \cup Y}(V_i) > 0\} \\ \text{i.e. } \#V_i \in Z \end{cases}$

A hetero-citation is defined here as a reference to a paper not belonging to the same corpus as the citing paper, which translates in the two corpora case featured in equation (4.1) as an edge linking a vertex from corpus X only ($V_i \in X^*$) to a vertex from corpus Y ($V_k \in Y$); $E_{V_i \rightarrow V_k}$. The hetero-citation share $S(V_i)$ of a publication represented by vertex V_i is the number of citations from V_i to corpus Y , $N_Y(V_i)$, divided by the total number of references from V_i , $N_{X \cup Y}(V_i)$. S_X then represents the mean share of hetero-citations per publication in corpus X , i.e. the average hetero-citation share $S(V_i)$ calculated over all vertices $V_i \in X^*$. Values close to 0 (or 1) mean that papers in corpus X cite mostly papers within X (or outside of X resp.). References to papers belonging to both corpora concurrently are counted as hetero-citations.

As large differences in size of the corpora X and Y can bias the metric S_X , the hetero-citation balance D_X , which I defined as the deviation of the observed S_X from the ideal value expected in theory in the absence of community-based clustering, was also

calculated:

$$D(V_i) = \frac{S(V_i) \cdot n_{X \cup Y}(V_i)}{n_Y(V_i)} - 1 \quad \text{and} \quad D_X = \frac{1}{n_{X^*}} \sum_{V_i \in X^*} D(V_i), \quad (4.3)$$

where $n_Z(V_i)$: number of vertices in a given corpus Z at the time V_i appeared, i.e. $\#V_u \in Z \mid \text{Year}(V_u) \leq \text{Year}(V_i)$.

The rationale underlying this metric is that, when X and Y form a completely unified discipline inside which authors are acquainted with all publications, irrespectively of the corpus they belong to, papers include a share of references to each corpus consistent with the latter's relative size. For example, if corpora X and Y comprise 2000 and 500 publications, respectively, they should represent 80% and 20% of the relevant citations per paper on average. A deviation from this expected frequency indicates a violation of the foregoing premise, the nature and extent of which is appraised through the sign and absolute value of D_X . For example, if $D_X = -0.5$, papers from corpus X cite on average 50% less papers from corpus Y than they should. Moreover, a comparison over time of hetero-citation share and balance reveals the force driving changes in mutual awareness among communities by disentangling the effects of relative community growth and publication- or author-level increase in hetero-citation.

The significance of hetero-citation balance D_X values was assessed through Monte Carlo randomization, which consisted here in the creation of 300 graphs with the exact same topology as the observed one, but with a random reattribution of corpus for each vertex. D_X was then computed for each of these graphs, providing a null probability distribution. Glass' estimator of effect size was then calculated to assess the extent to which observed values deviated from the null distribution [53]. The separation of the ABM and IBM corpora was thereby verified to be highly significant (Glass' $\Delta < -15$).

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(c) Identification of key papers

In order to identify which papers initiated the fusion of ABM and IBM research, a first stage inspection (see the electronic supplementary material, Extended methodology) was reassessed formally by the computation for each vertex of a quantitative metric, J_i , that evaluated how much a publication drew interest from both corpora concurrently (i.e. to what extent it was cited jointly in the ABM and IBM corpora). For this purpose, for a given publication, V_i , the minimum between the number of its citations stemming from each corpus was extracted:

$$J_i = \min(\deg_X^-(V_i), \deg_Y^-(V_i)), \quad (4.4)$$

where $\deg_Z^-(V_i)$: number of citations to V_i from corpus Z , i.e. $\#E_{V_k \rightarrow V_i, V_k \in Z}$. J_i was complemented with the calculation of BC, a metric that conveys the capacity of a publication to control the flow of citations in the whole network and, hence, its contribution to network connectivity [54].

Further methodological points are described in the electronic supplementary material, Extended methodology.

Data accessibility. All data necessary to reproduce this study are provided as the electronic supplementary material and on Dryad [55].

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