Alternative ways of verification and validation of computational models: A case of replication in the innovation networks

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Abstract

Conventional practice in modelling requires checking that the model implementation is correct with respect to its conceptualisation (verification) and that corresponds to and explains the real world phenomenon modelled (validation). Agent-based models (ABM) have been applied in many scientific fields, but only recently researchers have started to realise that the lack of verification and validation protocols/approaches is one of the main challenges and criticisms in fully adopting the models. Verification and validation assure the external and operational validity of a model and when data for estimation is not readily available, the behaviour of the computational model cannot be operationally validated and thus, the results are 'questionable'. Alternative approaches have recently gained increasing attention. Docking or replication of the models is one of them, based on the reflection that if different implementations of a conceptual model produce similar findings, that lends support to the models in mimicking the real world phenomenon.

This paper reports on the docking experience (using fuzzy logic) and other approaches to validate an agent-based model (ABM) in the context of innovation in business networks. Using two modelling paradigms and software programs, we modelled in 18 months' interval a network of three categories of agents (R&D organisations, venture capitalists VCs, and manufacturing companies M). The two models were developed for exploring innovation creation and change of resources in business networks. Agent-based and fuzzy logic approaches capture inter-relations between heterogeneous organisations/agents and between organisations and their environment, and cumulative network effects explain changes in the system. The organisations are autonomous and they exchange resources in a decentralised manner, the result in the system as a whole being dependent on the degree of interdependence of agents in the network.

Keywords: Validation, Replication, Docking, Innovation networks

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1 Introduction

Agent-based models (ABM) have been increasingly applied in recent years in social sciences. The range of simulation applications is large and varied (Bankes, 2002; Midgley et al., 2007) as simulation modelling has shown "the potential to be more sophisticated, subtle and faithful to the complexity" than the more traditional methods (Midgley et al., 2007: 884). Although development of simulation is now easier for those without extensive technical skills and the benefits have been demonstrated, agent-based simulation has yet to emerge as a commonly accepted research method/standard tool (Richiardi et al., 2006; Midgley et al., 2007). And the lack of standards for validation and verification is one of the main hurdles for their adoption ("quality assurance, especially correctness and validity of models and of modelling results becomes a major concern" - Wang and Lehman, 2007). Hence, for agent-based simulation models to become mainstream research approaches and realise their scientific potential, further work needs to be conducted into how models are validated and verified (Cioffi-Revilla, 2002; Maguire et al., 2006; Richiardi et al., 2006).

Proof that an ABM model is correct is in general difficult, as for these models traditional validation methods are not always applicable (Wilensky and Rand, 2007; Louie and Carley, 2008). However, as Louie and Carley (2008) have recently stated, these models "should not be considered an inferior method for studying social systems because familiar statistical techniques cannot be applied to validate all parts of the model" (p.252). The simulations are useful; the question is to understand their usefulness.

We found similar arguments in the papers by Robinson (2002), Midgley et al. (2007) – consistency in results, predictions from different models can be used to support validity of models and enhance credibility (confidence placed in a model and its results) and usage; statistical validation, although useful, should not be seen as providing the "absolute" validity of the model (Robinson, 2002).

Besides the fact that ABMs are relatively new in the modelling arena and a standard has not been set as such, the main reasons researchers miss out on validating and/or verifying their models include: considerable time and effort required to undertake the processes, with many replications not successful (Maguire et al., 2006); insufficient description of the models making replication impossible (Richiardi et al., 2006); differences in the interpretation of the theoretical underpinnings (Maguire et al., 2006); difficulty in applying models to real-world situations or impossibility to obtain real data and thus undertaking empirical validation (Wilensky and Rand, 2007).

In response to this critique/concern, a number of researchers highlighted the need to develop a suite of "best practices" allowing them to validate and verify the computational simulation models they develop (Wilensky and Rand, 2007:6; Richiardi et al, 2006; Louie and Carley, 2008; Wang and Lehman, 2007; Windrum et al., 2007). Such practices are critical if computational simulation models are to be accepted by the wider academic community and their findings are to be used by practitioners (Maguire et al., 2006; Louie and Carley, 2008).

This paper presents a docking/replication validation procedure conducted between a fuzzy logic model (FL) and an agent-based model (ABM) and other approaches to simulation validity. The paper focuses on the research gap concerning the lack of validation processes outlined in the literature and the use of model docking as a validation process (Axtell, 1996). Replication standard holds that sufficient information exists to understand, evaluate, and build upon a prior work, so that results can be replicated without any additional information. In our case, the same researchers built the two models for exploring innovation creation and change of resources in business networks within 18 months, making the replication effort less arduous.

The structure of the paper is: following this introduction, Section 2 briefly presents several aspects of innovation considered in the study, Section 3 details the motivation for adopting ABM and FL, and Section 4 describes the built models. Section 5 is dedicated to validation and calibration and Section 6 presents the results and findings. The paper concludes with limitations and flags avenues for further research.

2 Characteristics of the innovative systems

In this paper we embrace the view that innovation = "successful exploitation of new ideas" (Gilbert, Pyka, and Ahrweiler, 2001). Each actor/agent has a knowledge base (internal resources) that can be used to generate (be converted into) innovations or has financial resources to leverage the creation of innovations using external resources (Gilbert et al., 2001). This definition assumes the existence of a *network* as the medium for generating innovations, rather than a maverick agent engaged in R&D and with sufficient financial resources to bring the innovations to the market for their adoption. Innovation is seen as a collective endeavour where networked agents, engaged in various enterprises work together to innovate and in consequence bridge the gap between resources and applications. *In other words, the innovation is not in the agents or relationships between them, but is the network of agents* (Watts, 2004).

This connectionist, affirmative post-modernist, post-structuralist, positivist ? view (Maguire et al., 2006) has been well reflected in Open Source movement (Bonnacorsi and Rossi, 2002) or Sillicon Valley clusters (Zhang, 2003) where collective action and coordination, in the absence of central authority, lead to innovation creation and diffusion. As indicated, we deem this approach in our research appropriate as we deal with a complex system, where autonomous agents interact dynamically in a non-linear fashion with emergent consequences (spillover effects).

The innovation network is made up of firms/organisations of different sizes, knowledge conditions, and innovation strategies within a specific industry, with a positive correlation between entry and exit rates (Herbert, 2006). *In our models the agents invest time/money and knowledge for creating new knowledge and the successful innovation depends on how the capital stock is exchanged with knowledge.*

In terms of factors determining processes of innovation and their relative effect, the evidence is inconclusive, and more research is required. Vega-Jurado et al. (2008) investigated factors contributing to product innovation in various industries and found that the firm's technological competencies (derived from in-house R&D) are determinant for innovation. Mixed results were found with respect to the role of the size and structure of the market/network; each firm's competencies (technological, measured by R&D intensity; knowledge and skills; organisational) determine the degree of efficiency with which the firm performs functional activities and affect its innovation behaviour.

Potential reasons for these diverse results include: nature of the innovation (radical vs incremental), technological intensity of the industrial sector (low vs high tech), characteristics of the firm, and the geographical region (Souitaris, 1999; Vega-Jurado et al., 2008). Cohen and Levinthal (1990) and Veugelers (1997) also pointed out that interactions between external sources of knowledge and in-house R&D may stimulate rather than substitute for firms' own R&D. The internal activities not only contribute to the generation of new knowledge, but also enhance the ability to assimilate and exploit knowledge generated outside. In an extensive literature review in diffusion of innovations in health services, Greenhalgh et al. (2004) found that size of the organisations act as a proxy for technology readiness/absorptive capacity for new knowledge, functional differentiation and resources to channel into new projects and that the "structural determinants of innovativeness interact in a complex, unpredictable, and nongeneralizable way with one another" (p. 606). *In this research we use the size of the agents to "allocate" resources that enable them to interact for innovation creation.*

Vega-Jurado et al. (2008) also reviewed concepts such as the technological opportunity (probability that the resources dedicated to the development of innovation processes will generate real technological advances) and appropriation conditions (firm's capacity to retain benefits derived from innovative activities) as determinants of innovation.

When analysed within their environment, innovation networks are more durable and interactive compared to market links and this is a result of the trust, shared understanding of problems and objectives, acceptance of common rules and behaviours (Trippl and Todtling, 2007).

Many of these elements have been incorporated by Gilbert et al. (2001) in their innovation model, where the knowledge of an agent is represented by a 'kene', a triplet including technology capability, a corresponding specific ability, and the level of expertise of the agent. The agent gets a research direction via random selection of a set of triplets from the kene, and its expertise increases if abilities are used in the research, and decreases otherwise. Agents can change their kenes in the interaction with another agent from the network and innovation is successful if the accumulation of financial rewards exceeds a threshold. *Our approach differs by considering interaction between agents and characteristics of agents that are fuzzy and uncertain.*

A number of important areas in innovation networks have been identified as insufficiently explored: definition and operation of an innovation network, similarities and dissimilarities between innovation in different industries, dynamics of innovation networks (Gilbert et al., 2001).

This research addresses part of these questions applying two modelling approaches considered suitable for the characteristics of the innovation.

3 Agent-based modelling and fuzzy logic

Before describing the models we succinctly enumerate the main features/strengths of the two modelling paradigms we regarded as essential for our problem. We focus more on the ABM, as the fuzzy logic underpinnings have been described in detail in Purchase et al. (2006).

Agent-based modelling (ABM) is an alternative to classical thinking where systems' evolution is expressed using functions, equations, and algorithms. ABMs operate with agents, environment, objects which interact with each other. In addition to providing a natural and intuitive description of the complex[1] system, ABMs capture emergent behaviour (Bonabeau, 2002; Watts, 2004; Barnaud et al., 2008): the aggregated behaviour of a system is not the magnification of single agent behaviour at a larger scale.

ABMs "show how simple and predictable local interactions can generate familiar but enigmatic global patterns, such as the diffusion of information, emergence of norms, coordination of conventions, or participation to collective action." – Macy and Willer (2002: 143). This means entities endowed with certain behaviours and interactions lead to complex spontaneous dynamics in the system and large changes could be driven by even subtle modifications maybe imperceptible to actors having only local knowledge of the network (Windrum et al., 2007). "ABMs overcome an assumption that underlies much of the cognitive sciences that the individual is the crucial unit of cognition" (Goldstone and Janssen (2005: 424). In the same frame of mind, Pyka and Fagiolo (2005) emphasise the ABM's benefits of showing how the micro-level interaction leads to the genesis of collective phenomena and how to identify agents and behaviours with greater impact into the collective result.

ABM can handle a variety of heterogeneous adaptive agents with various behaviours who influence each other in response to the influence they receive. ABMs are very amenable to data-driven modelling without the need for gross aggregations and averaging (Macy and Willer, 2002).

The widespread of ABM in many fields is a response to the complexity of the real world phenomena and data availability and increased computational advances have facilitated it (Pyka and Fagiolo, 2005; Louie and Carley, 2008). ABMs are now present in market economics, supply chains, monitoring of industrial processes, geography, history/archaeology, epidemiology, biology, chemistry, defence applications, traffic management, land use, emergency evacuation (Bonabeau, 2002; Gilbert, 2004; Goldstone

[1] Complexity is used here in the technical sense that the "behaviour of the system as a whole cannot be determined by partitioning it and understanding the behaviour of the parts separately, which is the classic strategy of the reductionist physical sciences" – Gilbert (2004):3.

and Janssen, 2005; Macal and North, 2006; Purchase and Olaru, 2006; Rahmandad and Sternman, 2008).

Fundamental characteristics of the ABM regard (Macy and Willer, 2002; Tesfatsion, 2002; Windrum et al., 2007):

- Autonomy of agents – agents make independent decisions and the system is not directly modelled as a globally integrated entity, but self-organising patterns dictate the behaviour of the whole; the actors are interconnected elements that work together and the group level behaviour emerges without leaders ordering the processes (Bonabeau, 2002; Tesfatsion, 2002; Goldstone and Janssen, 2005);
- Interdependence of agents – direct and via environment, network; agents change their resources and the strength of their relationships with similar type of agents and with other classes in order to avoid becoming isolated in the network; the collective action result depends on the structure of the network (Watts, 2004) and the emergent structure is at a higher level than the individual (Gilbert, 2004; Windrum et al., 2007);
- Simple rules – global complexity does not necessarily reflect the cognitive complexity of individuals; ABM explore the simplest set of behavioural assumptions required to generate a macro pattern of interest; Bonabeau (2002) posits as a virtue of ABM the ability to exhibit complex patterns, unanticipated, even for simple ABMs;
- Adaptive/flexible behaviour – "agents adapt by moving, imitating, replicating, or learning, but not by calculating the most efficient action" (Holland, 1995:43, cited in Macy and Willer, 2002:146); agents use heuristics, adaptation, 'evolution'/learning to change their strategies (Goldstone and Janssen, 2005); Windrum et al. (2007) argue that agents should be assumed to behave as bounded rational entities with adaptive expectations;
- Dynamics nature – always in motion (Bonabeau, 2002; Gilbert, 2004); the state of the system is path dependent and by definition out-of-equilibrium (Pyka and Fagiolo, 2005; Windrum et al., 2007).

Macal and North[2] (2006) add another agent characteristic to this list – being goal-directed, having objectives to achieve with respect to its behaviour. In addition, Goldstone and Janssen (2005) emphasise the spatial dimension as the place where agents are and live/feed (environmental patches).

Srbljinovic and Skunca (2003) summarised some specific modelling advantages of ABMs, relevant in the innovation networks context: i) possibility to model more "fluid" or "turbulent" conditions and ii) to embed boundedly rational agents, making decisions with incomplete information; iii) ability to model processes out of equilibrium; iv) possessing unambiguous mathematical and computational formalisms.

Unlike simulation where traditionally structures are viewed as hierarchies shaping individual behaviour from the top down, ABM has a bottom-up approach (Macy and Willer, 2002; Pyka and Fagiolo, 2005). But, similar to simulation, ABM can be used to aid intuition, combining deduction (it has a set of explicit assumptions and initial conditions) and induction (generates data that can be analysed inductively to find patterns) treats. Macy

[2] Macal and North (2006) presented a tutorial on how to model with ABM. Valuable is the discussion on what makes an agent (pp.73-74) and the links of ABM with other modelling tools.

and Willer (2002) reviewed ABMs of emergent structure and order in papers published in sociology between 1997-2002 and concluded that ABM are most appropriate for studying processes that lack central coordination (Macy and Willer, 2002), which is the our case as well. Boulanger and Brechet (2005) found ABM as the most promising technique to deal with sustainable development issues when compared with six main families of modelling techniques including macro-economics, system dynamics, Bayesian statistics. Garcia (2004) affirmed that higher heterogeneity of agents in a system, greater impact of network effects, more adaptive/evolving the system make ABMs more suitable and effective modelling tool.

To conclude this preamble on ABM, we expand Axelrod (1997)'s statement that simulation is a "3rd way of doing science" (pp. 24-25) by suggesting that ABM is a 3rd way of doing science, with the benefit of linking micro-scale behaviour to the macro-scale behaviour of the system, but without aggregation.

The second modelling approach is fuzzy logic (FL), which provides an ideal framework to deal with independent layers of data of varying degrees of uncertainty/confidence, 'imprecision', membership (Zadeh, 1965). FL is another paradigm departing from traditional mathematical approaches and opening the door to a new way of defining knowledge using statements that can be true to a certain degree. Born to deal with degrees of truth (instead of the binary Boolean logic), tolerant to 'ambiguous', noisy data, and operating with linguistic expressions for reasoning, FL started to spread in numerous domains in the last decades (Cordón et al, 2001; Purchase et al., 2006). The mathematical set theory and logic are augmented in FL by making fundamental changes to the ideas of set membership and to the logical operations (Olaru and Smith, 2005).

The motivation for FL is provided by the need to represent propositions such as:

- Agent 13 and agent 7 are close friends.
- Most R&D do not have very high financial resources.
- Current market conditions are not favourable.
- This information is not relevant at all.

While traditional set theory defines membership as being either being true or not, FL allows us to represent set memberships with degrees of truth. The reasoning system is based on techniques that combine those membership functions using IF-THEN rules of behaviour. There are several structures of the fuzzy systems (including fuzzification interface, inference engine, knowledge base, defuzzification), but in this paper we use the Mamdani fuzzy rule based system (Cordón et al, 2001).

Each rule has a number of inputs/antecedents and one output/result. An example of a rule for our innovation model is:

IF (type of actor = "VC") AND (proportion in the network = "medium") AND (financial resources shared = "medium") AND (knowledge resources shared = "medium") AND (relational strength = "high") AND (relevance of knowledge resource = "high") AND (growth of resources = "power") THEN changes in network resources = "increase".

4 Model structure

Our purpose is to model changes in the information/knowledge and financial flows within a business network with actors interested in innovation. This is a symbolic network (Watts, 2004) where links describe abstract relations between agents collaborating for sharing new ideas and advancing technologies and the model identifies what drives processes of innovation. A range of behaviours is demonstrated in the network, from unequal distribution of resources and interaction function differences. The dynamics of innovation involve important characteristics of complex systems, which justify the ABM and FL modelling approaches (agent heterogeneity, non-linear interactions, network effects, stochastic elements and uncertainties).

We started out by defining the system, states, and input variables and parameters:

- *Types of actors* with relevant roles in the innovation network; VC, manufacturers, and R&D companies; these actors/organisations have different sizes, characteristics, and roles; they interact/share resources/collaborate for adoption and diffusion of new ideas that fit with the organisations' goals;

- The *attributes* relevant to actors and the behaviour exhibited by them (vector of characteristics); 100 actors (initially fixed population) are randomly generated in the network (random x,y coordinates) and they are then fully connected; the ties can be strong or weak (depending on how long the agents have been in contact to each other, the reciprocal/mutual services and amount of joined activities they have) and through them money and information flow (knowledge is particularly important for innovation, therefore knowledge providers are driving forces of innovation, generators of new innovations and promoters of external sources of scientific knowledge); spreading of the agents tends to reduce the intensity of the interactions in the network via a gravity function moderating the links parameters (Gilbert and Tierna, 2000);

- The *interactions* between actors embed a myriad of dimensions and are represented in the rules; if dissecting the links, we identify information processes, communication, collective learning, coordination of resources, all necessary to foster creation of new ideas; barriers to innovation are not exogenously introduced in the model (Goldstone and Janssen, 2005 suggest that ABMs control the ensemble without instituting barriers, which is fundamentally different from the most common method of controlling through direct orders, laws, rules); a threshold value of relationship strength (for example trust built over time in stable relations) dictates when actors can interact (below that value the relationship "dies") and depending on the resources they can put together, there is scope for innovation or otherwise; R&D activities require monetary resources and reduce the capital stock of the VCs or manufacturers, but the capital will be refreshed by successfully introducing a further innovation (considerable increase in the knowledge and skills);

- *Autonomy* is ensured by the dyadic approach to model interactions; the agents have local, micro-knowledge and do not know what happens within other relations but theirs, hence their decision is independent of other actions in the network; each run, agents interact with each other, share resources, collaborate, depending on their resources and the strength of their relationships (local information); the interaction/collaboration does not involve selective search for potential partners (as in Gilbert et al., 2001), interaction being a stochastic element;

- *Granularity and time horizon* for the problem analysed; the model evolves in discrete steps and at the end of one run/iteration, the actors will assess their resources and position in the network;

- *Environment* – industries/regions without tradition in innovation are likely to take a different route to innovation adoption and diffusion compared to high technology and speed clusters (Trippl and Todlling, 2007); highly competitive and dynamic environments affect the speed of innovation (e.g., IT, nano technology) – but this is not included at the moment in the model.

The ABM model is built in NetLogo 4.0. As indicated, in the initial network of 100 actors, the interaction/collaboration is not forced by the structure of the social ties, because their strength can be manipulated and even reduced to 0 (thickness of lines in Figure 1 suggests the strength of interaction). Agents possess various capabilities (deterministic and stochastic elementary properties) and we use link parameters to tune the degree of interaction between them. After specifying the behavioural rules for agents and for their interaction, we explore the consequences at the level of the network. The macro-variables contain the information relevant to the analysis of the system: averages of financial (F) and knowledge (K) resources, change in the total resources (I).

Initially, each type of actor VC (N1 actors), M (N2 actors), and R&D (N3 actors), has a certain amount of financial and knowledge resources allocated, based on their profile and size (F^0 and K^0 for each actor). As a result of the interaction (resources put together, strength of relationships, environment conditions), these resources are multiplied or depleted, converted into innovation so as at the end of a number of iterations the network "produces" new knowledge (the individual resources become F^f and K^f).

The fuzzy logic (FL) model has the same structure, but the inputs are fuzzified, then subject to the knowledge base with rules for operation in order to infer the changes in the network. The knowledge base includes 486? "IF-THEN" rules expressing the expert field knowledge of the authors. The multiple antecedents were connected by AND, OR, NOT operators and hedges. Multiple rules fire at the same time and they may have various weights.

The FL model is not a micro-scale model, and the results are reflecting the behaviour of the clusters of agents. With FL, we have had the possibility to address growth in a comprehensive manner, including a range of fuzzy factors: the fuzziness about what the agent or innovation really is, the fuzziness of antecedents of innovation and the interactions between agents. The model was built in CubiCalc 2.0.

The innovation system we map is presented in Figure 1.

State of the system/network at t_0 State of the system/network at t_f

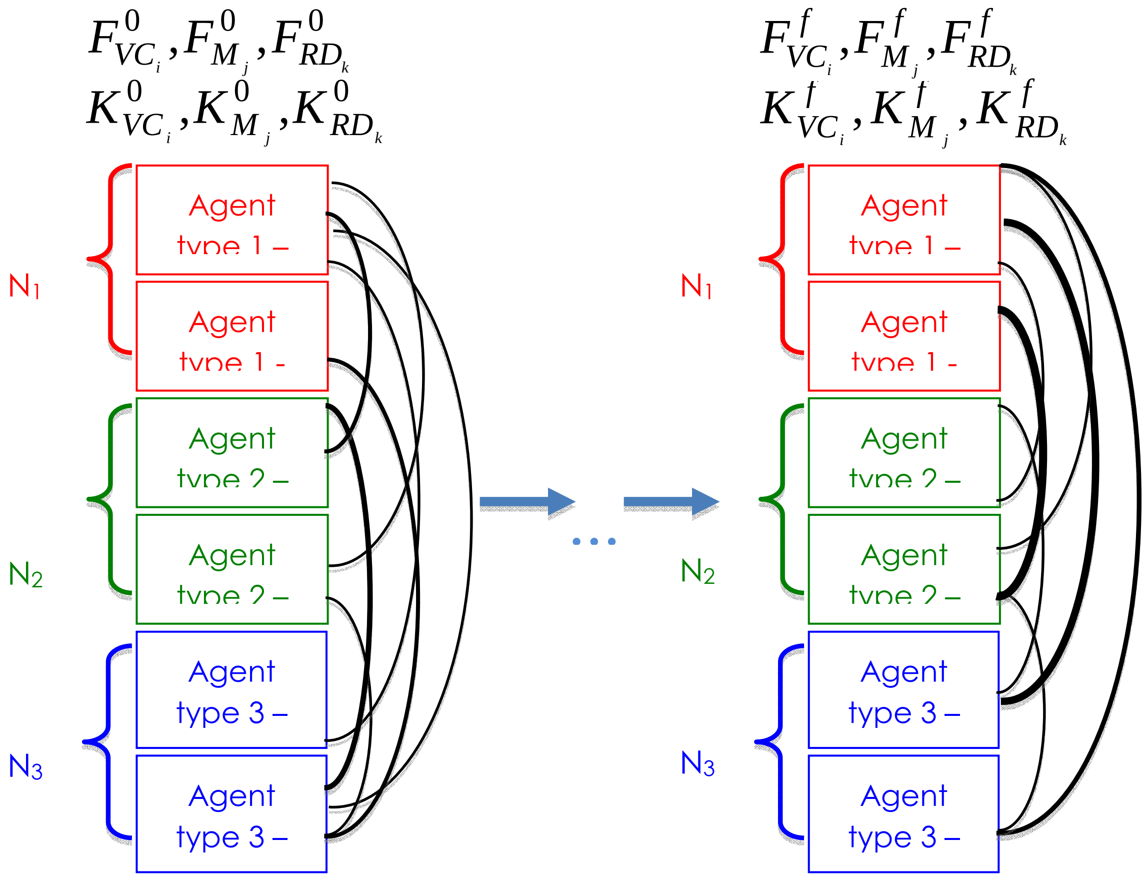

Figure 1 Components of the model and time dimension

The models do not make any distinction between incremental and radical innovations, do not consider speed of innovation nor incorporate rivalry with other agents, and are built for a specific industry (homogeneous in the culture of innovation). These boundaries of the models, showing what is left out of the modelling exercise, may limit the transferability of the findings across industries.

5 Validation and calibration

A recurrent problem in simulation is the evaluation and assessment of model quality. In our case, because experimental observations were not available, we searched for alternative ways to assess the validity of the predictive capabilities of our models.

Many researchers have recently addressed the validation standard and suggested avenues for eliminating the most common criticisms brought to simulation models – that of not been demonstrated as correct. Richiardi et al. (2006) highlighted a framework for validating agent-based models. The framework includes: theory validity; model validity; program validity; operational validity; empirical validity; structure verification; extreme condition and boundary adequacy. Within the framework of validation a number of different techniques can be used, with some techniques covering more than one category of model validation. This paper concentrates on *docking* (Axtell et al., 1996) and *sensitivity analysis* (Wilenski and Rand, 1997; Louie and Carley, 2008) for model validation. Other techniques for validation and verification that are not addressed here include: developing simulation rules from existing rich theory such as case studies; indicating that the patterns of model results are consistent with real-world processes, through methods such as case analysis; discourse analysis and action research (Richiardi et al., 2006; Maguire et al., 2006).

Axtell et al. (1996) developed the basic concepts and methods of docking (to explore how alignment of the results of one computation simulation with the results of a replicated model can assist model validation). It should be noted that replication differs from model re-implementation (re-writing code) and that docking only refers to model replications (the model being re-written with different mechanisms or processes used to conduct the simulation). Replication assures the researcher that the model outcomes are stable (repeatedly generated) and not produced by exceptional circumstances (Wikensky and Rand, 2007) and thus it allows the researcher to establish an indirect relationship between the theoretical underpinnings of the model and its results.
Replicated models differ across six dimensions: time; hardware; languages; toolkits; algorithms and authors (Wilensky and Rand, 2007), with the different mechanisms being the most important aspects of replication (Axtell et al., 1996).

However, replication alone is not sufficient for validation. Criteria are required to delineate the extent of replication achieved and the equivalence of the results. Axtell et al. (1996) gives three categories for assessing docking: numerical identity, distributional equivalence, and relational alignment. Numerical identity suggests results that are numerically the same in the two models. Distributional equivalence considers that the distributions of results are statically indistinguishable. Relational alignment highlights that the patterns of interactions in the models as the same across the two models (Axtell, 1996).

In the innovation network models, the validation involved several stages, presented in Table 1:

Table 1 Validation approaches and stages

Conceptual validity – based on theories	Structure of the model is supported by literature (Denize et al., 2007)
Expert judgement – discussions with colleagues in various forums (seminars, conferences); as indicated by Gilbert and Troitzsch (1999) and Bonabeau (2002), validation of ABM of social processes inevitably assumes a degree of arbitrariness and subjective/expert judgement	On numerous occasions (IMP and ANZMAC conferences) we found confirmation for the representation of each dimension in the model and for the hypotheses included
Input validation – ensuring that the fundamental conditions incorporated in the model reproduce aspects of the real system	Ex ante - verification of the ranges of the parameters of the models (decay of irrelevant information, relativity between financial and knowledge resources for the three classes of actors
Believability test - checking the correspondence between what is emerging from the model and what is expected to be seen in the real world; although this is not sufficient for concluding that the models are correct, the fact that the model components adequately represent a real equivalent behavioural effect is	

of paramount importance when real data is not available at the time of designing the models Examples of judging the model output include: - a) effect of network density - b) analysis of extreme conditions – reducing to zero the resources for each type of actor	a) Network density creates clusters with enhanced ability to innovate, showing/confirming that geography is important; we emphasise the model does not generate a particular pattern of clusters, but the grouping that emerges displays the same "signature" – greater resources and innovation creation (Figure 3) Also, the smaller the network, the greater the probability for an actor to interact with a previous actor b) The network collapses according to the rules
Internal validity – comparing the results from simulations with various random seeds for assessing consistency - changing the type of the noise – comparing results from: - a) changing the normal distributions to uniform distributions and - b) changing the parameters of the normal distributions (Richiardi et al. , 2006)	Statistical tests confirm repeatability (no statistical difference between runs) Normal distribution of effects in all situations (Kolmogorov-Smirnov test)
Sensitivity analysis – what-if scenarios to ascertain the effect of inputs upon the model's output; we conducted sensitivity with respect to: network size, proportion of actors, strength of relationships	Sensitivity analysis revealed the most important effects and we invested to collect data in those fields. The hypotheses that guided the experimental design (behavioural space) are: - stronger ties between agents are associated with generation of new ideas and adoption of innovation if the relevant knowledge flows between R&D to users of innovation; - knowledge is "lost" if there is no good soil to seed it (at least moderate strength of interactions and resources to develop/implement the innovation); - imbalanced number/proportion of the three types of agents may hinder the realisation of new ideas (Figure 3); agents are a driving force of evolution of the innovation in the system, they respond to the environment, and are engaged in goal-directed behaviour, but they need access to resources to interact; endowments are crucial assets of agents in accomplishing their tasks (Pyka and Fagiolo, 2005); - environment conditions – boom or financial turmoil moderate the network

	effect. Proportion of actors and higher density network are sensitive inputs: imbalance in the number of actors of all types (extreme condition tested – type of actor missing) leads to disfunctionalities in the network; smaller and denser networks (50 actors) display higher levels of innovation compared to larger networks (100, 200 actors)
Docking – comparing the results of the two different modelling approaches (Axtell et al., 1996; Xiang et al., 2005; Purchase et al., 2008). Over 1,000 runs for the fuzzy logic model and over 5,000 runs for ABM	The models ensure distributional equivalence, but they are not identical, as it is impossible to get numerical identity given the two distinctly different simulation mechanisms used. Both models used the same parameters, so we believe that the differences in results arose only from relaxing the restrictive assumptions in the FL or ABM models. Fuzziness was not possible in the ABM while emergence and extended time periods were not possible in the fuzzy logic model. The stochastic ABM generates a distribution of outcomes caused by random encounters among agents, while FL generates an ensemble of crisp values as result of multiple rules of interaction applied simultaneously. Both simulation models produced three clusters: awesome, steady, and vulnerable. Cluster profiles are similar in the two data sets. The "awesome" cluster includes actors with higher level of knowledge resources and relevance of those resources, with stronger ties/collaborations with other actors, therefore a more privileged position in the network. This cluster includes the highest proportion of R&D companies, the generators of knowledge. The "vulnerable" cluster comprises actors with low level of knowledge resources and weak ties; whereas the "steady" cluster has a mix structure in both models. MANOVA highlighted that the clusters are associated with statistically different measures of resources, relations, and change, but the type of model did not have a significant effect on the results. The results indicate a high level of equivalence. Such differences were recently found by Rahmandad and Sterman (2008) who compared ABM with differential equation models using epidemic spread as example. The means for several metrics were distinct between models, as well as the responses of the models to policies.

Following Louie and Carley (2008)'s types of validation, we addressed the conceptual validity, and partly the validity of data and operational validity (extent to which the model output matches the real system for the purpose it was developed). The *conceptual validity* was assessed via experts, *data* via sensitivity to parameter changes, and *operational* via replication (Figure 2). The two dotted lines indicate techniques for operational validity not possible in our case with the usual empirical analysis. Replication instead supports the validity.

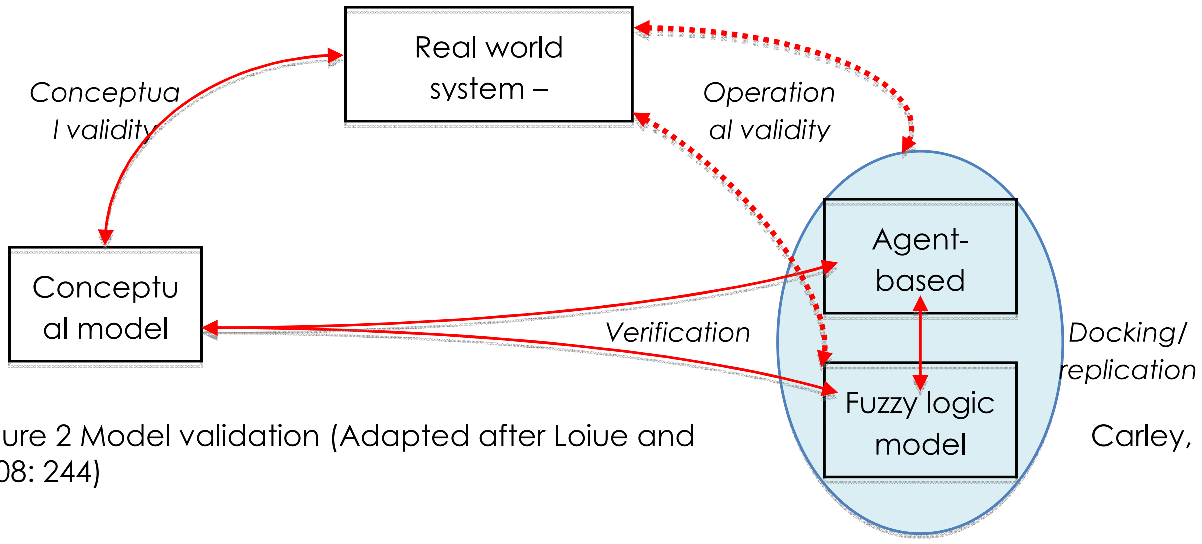

Figure 2 Model validation (Adapted after Loiue and Carley, 2008: 244)

6 Findings and conclusions

We go beyond mathematical modelling applying a more tractable approach – simulation. Our simulation is ABM, the third type identified Gilbert and Troitzsch (1999) in the development of social simulation, different from macro and micro-simulation, and newer than them. While macro and micro simulations use distributions, equations, and algorithms to model behaviour, ABMs explore interaction between agents. Our model is particularly useful to shed light on the relations between agent behaviour and the emergent behaviour of the innovation network, and to generate synthetic data under a variety of conditions to represent possible situations in the real world innovation networks. This is because ABM models enable us to examine questions not easily modelled by traditional approaches/representations, being a more realistic representation of complex dynamic systems. The outcome is more/different from the sum of the parts and the emergent behaviour cannot be understood without a bottom-up dynamic model. The ABM structure is flexible and tolerates combination/blending of various tools. The dilemma we faced was to trade-off the descriptive accuracy and the explanatory power (KISS vs KIDS problem described by Goldstone and Janssen, 2005:21), trying to identify the crucial real-world elements to drive the innovation in business networks in order to make the model tractable (Frenken, 2005).

In the same spirit as most ABM applications, we were more concerned with the theoretical development and explanation of phenomena than with prediction (Axelrod, 1997; Gilbert et al., 2001), therefore the lack of real data was not considered a hurdle for developing the models.FL and ABM models of the innovation network produce similar results. Both models used the same parameters, therefore differences in outcomes arose only from relaxing the restrictive assumptions in the FL or ABM models. The ABM results matched the FL conditions tested. The stochastic ABM generates a distribution of outcomes caused by random encounters among agents, while FL generates an ensemble of crisp values as result of multiple rules of interaction applying simultaneously.

Through replication, we gained confidence in the algorithms and implementation and the results are plausible. Within their domain of applicability, the models have a satisfactory range of accuracy and support our hypotheses on innovation creation and the stance that the empirical validation should not be the primary basis for accepting or rejecting a model. We also share the view expressed by Rahmandad and Sterman (2008) that the two models used in docking should be viewed as complementing each other, being "regions in a space of modelling assumptions, not as incompatible modelling paradigms" (p. 1001). The distinct modelling approaches provide complementary views on the mechanisms operating in the innovation networks. The further development of the ABM model (without equivalent in the FL though) emphasizes the importance of network effects in innovation networks. In addition, we applied sensitivity analysis to gain a deeper understanding of complex behaviour of the system as a whole. As Tesfatsion (2005) suggested, ABMs are a laboratory where we experiment numerous scenarios to assist model validity. Here, we manipulated the structure of the network and the parameters of the agents to see the implications at macro level.

With respect to model development, it is important to note that the models were incrementally developed, with ad-hoc adjustments arisen from theoretical base and discussions with peers in order to arrive at a better representation of the innovation network, to understand the factors and assumptions. Here we followed the recommendation made by Macy and Willer (2002): 162 that "models should start out simple and complications should be added one at a time, making sure that the dynamics are fully understood before proceeding". The incremental elaboration allowed for easier understanding and interpretation, fostering discussion and further exploration. This is crucial for practical significance if we want to bring evidence supporting the theory and allowing for action.

We conclude this section with some thoughts from Kleindorfer and colleagues (1998) in relation to various positions in the philosophy of science with respect to validation: in the simulation literature there is a continuum of opinions ranging from extreme objectivist (model validation can be separated from model builder and its context) to relativist ("model and model builder are inseparable" and "validity is a matter of opinion" – p. 1097). Their debate leads to a perspective that simulation modelling should not follow a prescriptive set of approaches to validation, but rather modellers should "responsibly and professionally argue for the warrant of the model."

7 Limitations and future developments

One of the difficulties in this docking case was that the ambiguity and uncertainty built into the fuzzy logic model was not possible in the ABM. The experimental generation of values in the fuzzy logic uses linguistic variables (low, medium and high) with membership functions, while the ABM required probability distributions for each of the variables.

Another difficulty is that the fuzzy logic model only gives results at the aggregate / network level while the ABM gives results at the individual level. To overcome this limitation the results of the ABM were aggregated to the network level. Such aggregation loses some of the interesting outcomes of ABMs, i.e. patterns of outliers would be lost in aggregation. Investigation of these different patterns at the individual level might produce further insight that is not possible in the fuzzy logic model.

With respects to model limitations, in this innovation network the adaptation is not based on evolution, and it does not involve competition for survival; we have not incorporated "copying" behaviour between agents and the likelihood of interacting with other actors is random and not determined by the similarity of the "cultural traits" of the actors. However, the rules are determining the changes in innovation and the actors can revisit their behaviour and alter current practices based on the "balance sheet" of their resources.
Another aspect worth investigating is the speed of innovation, highlighted by Kessler and Chakrabati (1998) as crucial for obtaining "pioneering advantages" (p. 1144). This must be corroborated with the environment characteristics and the industry depicted by the network: highly competitive and dynamic environments may trigger increases in the speed of innovation (e.g., nano-technology, mobile communications), whereas regulatory acts may temper the rhythm of innovation (e.g., GM for food, new drugs). Fast innovations generally require higher costs, therefore the results of an accelerated process would have to be re-casted in our ABM and fuzzy models.

Improvements to the models include:

a) incorporating a more strategic view of the goals a specific agent has; currently the three categories of agents are not "seeing over the fence", their visibility is reduced to one run;

b) incorporating how policies fostering/restrictive for innovation impact the innovation diffusion – based on case studies;

c) hybridisation of the ABM with fuzzy logic, in this research precluded by the programming abilities of the team members. Positive results have been obtained by Hassan, S., Garmendia, L., and Pavón (2007) who introduced FL in the ABM models in sociological analysis of family and friendship relations between humans.

8 References

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Appendix

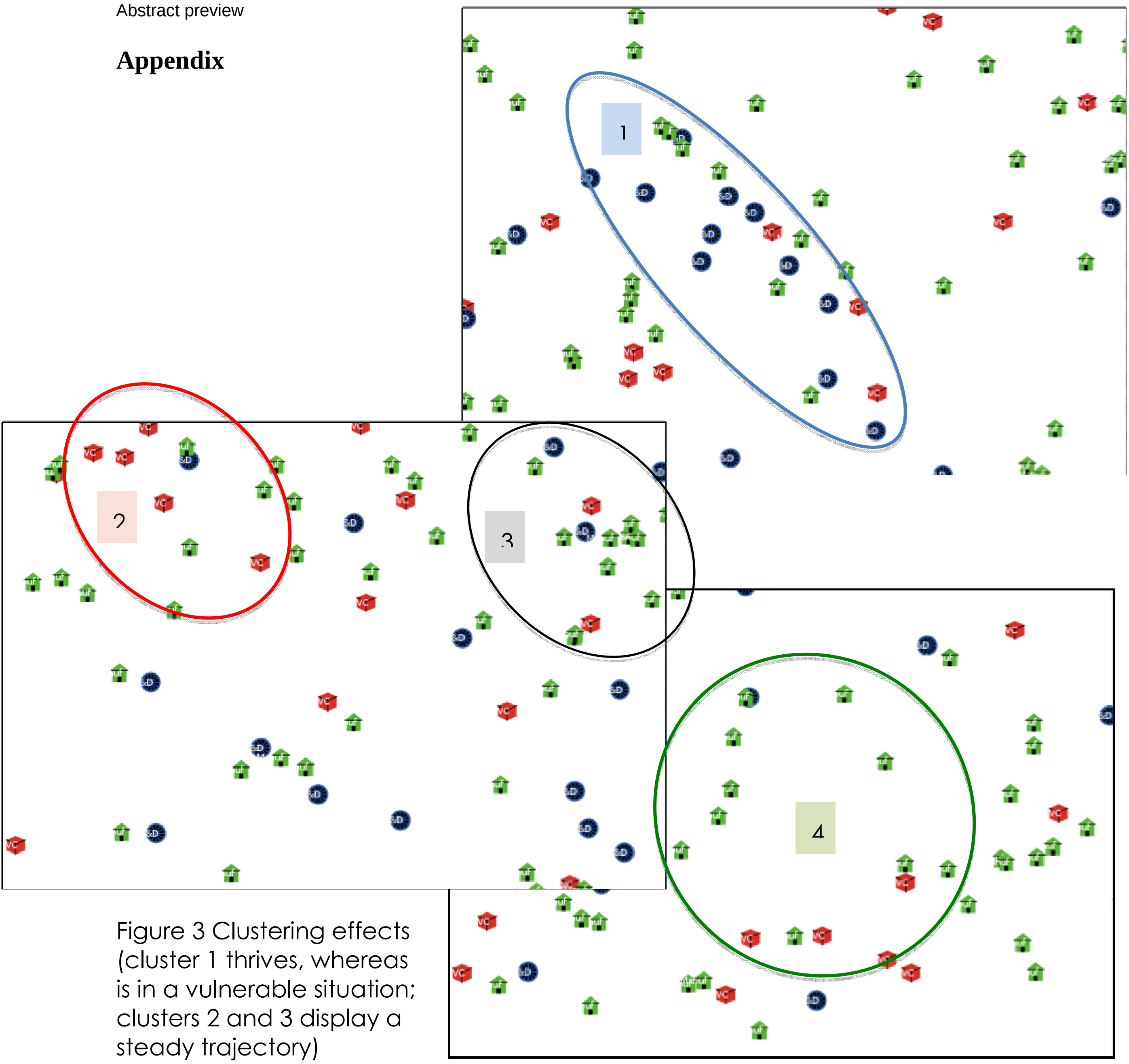

Figure 3 Clustering effects (cluster 1 thrives, whereas is in a vulnerable situation; clusters 2 and 3 display a steady trajectory)

4

N.B. The links were removed to enhance the clarity of the visual display