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Lessons from a comprehensive validation of an agent based-model: The experience of the Pampas Model of Argentinean agricultural systems

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ABSTRACT

There are few published examples of comprehensively validated large-scale land-use agent-based models (ABMs). We present guidelines for doing so, and provide an example in the context of the Pampas Model (PM), an ABM aimed to explore the dynamics of structural and land use changes in the agricultural systems of the Argentine Pampas. Many complementary strategies are proposed for validation of ABM's. We adopted a validation framework that relies on two main streams: (a) validation of model processes and components during model development, which involved a literature survey, design based on similar models, involvement of stakeholders, and focused test scenarios and (b) empirical validation, which involved comparisons of model outputs from multiple realistic simulations against real world data. The design process ensured a realistic model ontology and representative behavioral rules. As result, we obtained reasonable outcomes from a set of initial and simplified scenarios: the PM successfully reproduced the direction of the primary observed structural and land tenure patterns, even before calibration. The empirical validation process lead to tuning and further development of the PM. After this, the PM was able to reproduce not only the direction but also the magnitude of the observed changes. The main lesson from our validation process is the need for multiple validation strategies, including empirical validation. Approaches intended to validate model processes and components may lead to structurally realistic models. However, some kind of subsequent empirical validation is needed to assess the model's ability to reproduce observed results.

1. Introduction

Agricultural systems are complex systems, as they have multiple scales of interactions, are strongly influenced by human decision-making and include feedbacks with natural ecosystems. Agent-based modeling (ABM) is well suited to studying complex coupled human-natural systems (Hare and Deadman, 2004; Rounsevell et al., 2012). ABM is a powerful technique to assess system-level patterns that emerge from the actions and interactions of autonomous entities (Gilbert, 2008; North and Macal, 2007). This is the case of land use and structural patterns in agricultural systems, which emerge from individual farmers' decisions interacting with one another and an environment. Another crucial feature of ABM is the possibility of considering heterogeneity in, and interactions between individual components. Therefore, there is no need to assume "a representative farmer." Finally, ABMs provide a one-to-one mapping between real-world entities (e.g., "a farm") and their virtual representations (Rounsevell et al., 2012). This ontological correspondence, together with the fact that rules and behaviors are often expressed in readily understood natural language, facilitate the involvement of stakeholders in model development.

Agent-based models (ABMs) have been applied to a variety of problems in recent years (Heath et al., 2009; Heckbert et al., 2010). There is a vast literature on ABMs and land use changes; see reviews by Parker et al. (2003) and Matthews et al. (2007). Some examples of agricultural applications are described in Berger (2001), Berger et al. (2006), Happe et al. (2008), Freeman et al. (2009) and Schreinemachers and Berger (2011). As the use of ABMs has increased, there has been growing interest in the validation – i.e.,

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the process of assessing the level of confidence that can be placed in the model – of this particular type of model. However, although there is a vast body of literature on alternative approaches and procedures for validating ABMs, there are few published examples of comprehensively validated models (Bharathy and Silverman, 2013). In fact, many ABM efforts do not go beyond a "proof of concept" (Heckbert et al., 2010; Jansen and Ostrom, 2006). Difficulties for rigorous validation have been identified as a main frontier for ABM research (Heckbert et al., 2010).

The complex nature of agent-based models (ABMs) makes validation of these models challenging. ABMs are aimed at studying social-ecological systems where the fundamental underlying laws are not known or are unclear. ABMs almost invariably contain non-linearities, stochastic dynamics, non-trivial interaction structures among agents, and micro-macro feedback loops (Fagiolo et al., 2007b). Consequently, the system-level behaviors and structures generated by interacting agents often are difficult to predict. Furthermore, behavior can be extremely sensitive to initial conditions and show path dependency because of feedback loops (Rand et al., 2003). On the positive side, ABMs have the particular strength that they can be validated with respect to both qualitative and statistical data and at both micro- and macro levels (Moss and Edmonds, 2005). A recent summary of alternative approaches for validating ABMs is given by Bharathy and Silverman (2013).

The Pampas Model (hereafter, PM) is an agent-based model of agricultural production in the Argentine Pampas, one of the most important agricultural areas in the world (Calviño and Monzón, 2009). The development of the PM was motivated by the need to gain insight into the processes underlying recent structural and land use changes in the Pampas. The most significant changes have been: (a) an increase in the area operated by individual farmers, accompanied by a decrease in the number of active farmers, (b) an increase in the amount of land operated by tenants, and (c) changes in land use patterns, in particular, the increasing dominance of soybean. The PM was presented in detail by Bert et al. (2011). After the development of the PM, our research emphasis evolved from using it as a test bed to gain deeper insights into historical patterns, to exploring plausible future trajectories of agricultural systems in the Pampas. Consequently, we conducted a process of comprehensive validation of the PM to evaluate its ability to answer the questions it was designed to address (Rand and Rust, 2011).

In this paper we present guidelines for the validation of ABMs, providing an example in the context of the Pampas Model (PM). We describe the validation process of the PM and we share the main lessons learned from our attempts to perform a comprehensive validation of an agent-based model. The paper is organized as follows: First, we present a brief review of approaches for validation of agent-based models. Then, we present our validation framework, describing the various streams and strategies adopted and their main results; special focus is placed on results from multiple simulations aimed at calibrating the model and assessing its capability to reproduce the direction and magnitude of changes observed in the Pampas. Finally, we identify and discuss the main lessons learned during the validation process, in the hope that our experience may help others undertaking similar tasks.

2. Validation of agent-based models

Different frameworks have been proposed that combine multiple approaches to ABMs validation (Gürcan et al., 2011; Macal and North, 2005). Bharathy and Silverman (2013) recommended the triangulation of multiple validation techniques for a holistic evaluation of ABMs. Undoubtedly, using as many validation approaches as possible will enhance user confidence in how well a model works. Approaches to validation of ABMs may be grouped into two different, yet complementary, streams: (1) matching model components and processes to real-world components and processes, and (2) matching both simulated aggregate patterns to real-world patterns and comparing quantitative model output with measured variables. This multi-stream approach is analogous to the "cross-validation" proposed by Moss and Edmonds (2005), in which models are assessed independently at both the micro and macro levels (Rand and Rust, 2011). The following sections summarize the main concepts and strategies encompassed in each validation stream.

2.1. Validation of model components and processes

The first validation stream involves what Rand and Rust (2011) call "micro-face validation," that is, the process of making sure that the mechanisms and properties of the model correspond to real-world mechanisms and properties. The ability to replicate empirical evidence is often seen as the only truly decisive criterion for quality of a scientific model. However, most ABMs are used for the analysis of non-observable scenarios, such as the implementation of hypothetical policies or new technologies. By their very nature, there are no real-world data available for these situations. Therefore, the simulation model needs not only to be empirically valid, but also show theoretical validity, agent behavioral validity, validity under extreme conditions, and structural validity (Damgaard et al., 2009). All these characteristics contribute to the *conceptual validity* of a model. Conceptual validity can be assessed by determining the extent to which the chosen theories and underlying assumptions are appropriate for the purpose of the model.

Unlike the conventional validation, where a model is judged once it has been finished, validation of ABMs should start from the beginning of the modeling process, that is, the conceptual design stage (Macal and North, 2005). Effective model design principles can help mitigate some of the difficulties of validating ABMs (Edmonds and Moss, 2005). For example, the TAPAS (Take A Previous Model and Add Something) approach has been proposed for the design of ABMs (Polhill et al., 2010). This incremental modeling approach enhances the conceptual validity of new models by building upon previously used, well-understood and accepted models, components, theories, and underlying assumptions. Other design concepts – e.g., "modeling for a purpose" (Takama and Cartwright, 2007) – suggest guiding model design according to the aims of the model stakeholders. This approach also contributes to model validity, as the evaluation and validation process is fundamentally tied to the purpose and the context for which a model is being developed (Louie and Carley, 2008). Finally, model validity can be enhanced through the Pattern-Oriented Modeling (POM) approach proposed by Grimm et al. (2005). The central idea behind POM is using patterns observed in real systems to guide the design of model structure.

Participatory modeling – the engagement, collaboration or participation of stakeholders in model development – can be yet another important component of conceptual ABM validation (Barreteau, 2003; Voinov and Bousquet, 2010). This approach involves continuous adaptation of the model structure and processes based on feedback from stakeholders. Repeated interactions between modelers, domain experts and other stakeholders contribute to ensuring the validity and reliability of model structure, assumptions, processes and outcomes (Louie and Carley, 2008). Moreover, stakeholder participation not only contributes to model validation, but also to enhance the quality, transparency, credibility and relevance of the model (Voinov and Bousquet, 2010; Zellner et al., 2012). Involvement of stakeholders is not limited only to model development phases, but also may include running simulations. Participatory simulation, where real people play the role of agents, may serve to identify or validate key assumptions about agent behaviors (Ligtenberg et al., 2010; Macal and North, 2005).

Expert evaluations offer another way to validate models. Macal and North (2005) distinguish two types of experts: (a) those involved in the development of the model, and (b) independent experts (i.e., not closely involved with model developers) who review model assumptions and results. Feedback from both kinds of experts can contribute to ABM validation efforts.

2.2. *Empirical validation*

Many models, as representations of real-world systems, are evaluated by how well they can match the behavior of the target system – that is, comparing model output with real world observations. The second model validation stream, therefore, is related to empirical validation (Fagiolo et al., 2007a). *Empirical validation* is the procedure through which modelers assess the extent to which a model's outputs approximate reality. Reality is typically defined by one or more "stylized facts" drawn from empirical research (Fagiolo et al., 2007b). Windrum et al. (2007) and Moss (2008) discuss several alternative approaches to perform empirical validation of ABMs.

Empirical validation of ABMs may involve not only the assessment of the extent to which the model reproduces reality, but also simultaneous calibration, tuning and further development of the model. Windrum et al. (2007) describes alternative approaches based on empirical validation to identify sub-regions in the potential parameter space that lead to replication of relevant statistical regularities or stylized facts. Equally informative can be the identification of simulation conditions that invalidate the model (Macal and North, 2005) such as discovering cases for which the model behavior is outside of the range of what is expected. The testing, tuning and further development of an existing model can be guided by observed patterns that the model seeks to explain. Topping et al. (2012) refer to this process as "Post-hoc Pattern Oriented Modeling." They describe an example of how POM can be used for both model design and evaluation. In summary, the empirical validation of an ABM may focus on assessing the model's ability to reproduce observed patterns as well as calibrating and further developing the model based on these patterns.

3. A validation case study: The Pampas Model

In this section we describe the PM validation process. First, we briefly describe the PM. Second, we present the validation framework we implemented for the PM. Finally, we describe the set of strategies adopted as part of the framework and the main results from the validation process. We place special emphasis on results from simulations involved in the empirical validation of the PM.

3.1. *A brief description of the Pampas Model (PM)*

The PM is an agent-based model of agricultural production systems of the Argentinean Pampas. The PM was presented in Bert et al. (2011) following the widely used ODD (Overview, Design Concepts and Details) protocol (Grimm et al., 2006, 2010). Since then, we have implemented various refinements to the PM. Some of these modifications were motivated by the need to increase the fidelity of the model. The details are presented in Appendix A. Other modifications were identified as a direct result of the model calibration and validation process. These modifications will be discussed in the next sections.

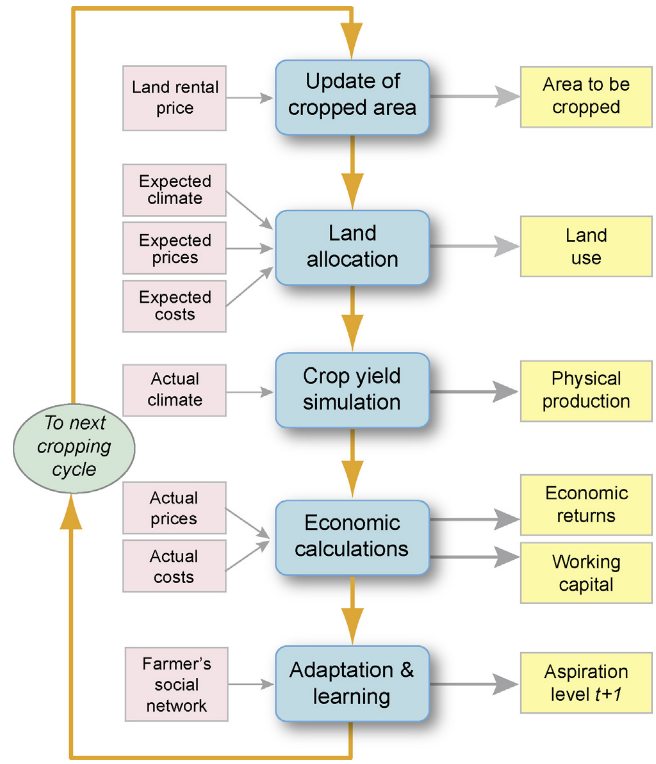

Fig. 1. Conceptual diagram of the sequence of processes for a single farmer in a production cycle. External context drivers are listed on the left of the diagram, and state variables associated with each process are shown on the right.
This figure was simplified from Bert et al. (2011).

The PM includes three main types of entities: the *environment*, *farms* and *farmers*. The environment represents the northern part of Buenos Aires Province, the most productive sub-region of the Pampas. This area encompasses about 1,000,000 ha and has a long agricultural history (Calviño and Monzón, 2009). The environment contains farms of variable size defined during initialization. All farms are assumed to have the same soil, namely Typic Argiudol, the most representative soil of the modeled region. All farms experience the same climate, which is represented by weather records from Pergamino, a location in the center of the region. Although the environment does not represent real geography, the model is spatially explicit because there is a topological relation among simulated farms that provides structure to interactions such as social comparisons or imitation. The model involves one main type of agent, farmers who grow soybean; maize; or a wheat and short-cycle soybean double crop on owned or leased farms. Each agent may have different land allocation strategies and financial (e.g., working capital) characteristics.

The main processes and sub-models included in the PM are shown in Fig. 1, redrawn from Bert et al. (2011). One model time step represents a cropping cycle from April to March of the following calendar year. At the beginning of each cropping cycle a farmer adjusts her economic aspirations based on the expected status of context factors (i.e., climate conditions, output prices, input costs). Then, through the "Update of Cropped Area" sub-model, the farmer decides whether she can (a) farm additional land, (b) maintain the same area as in the previous cycle or, instead, (c) must release some or all of the previously farmed area. In the current model, the only way to expand cropped area is by renting additional land. This is a reasonable approximation, as land sales in the Pampas are rare. Subsequently, the farmer allocates her land among a realistic set of activities: maize, full-cycle soybean and wheat-soybean double cropping.[1] After land is allocated, the yield of each selected activity is retrieved from lookup tables pre-calculated using biophysical crop models and historical climate conditions. Economic returns are (a) calculated from simulated yields and historical crop prices and input costs specified as model inputs, or (b) can be directly provided as input data. The end result of the economic calculations is an updated value for the farmer's Working Capital (WC) at the end of the production cycle. Economic returns are then assessed in relation to both the farmer's initial aspiration and her peers' performance. This assessment drives an adjustment to the farmer's Aspiration Level (AL). AL is a special value that separates outcomes perceived as successes or failures (Diecidue and van de Ven, 2008). This is used as an input to decisions in the following cropping cycle.

The PM is implemented in the Recursive Porous Agent Simulation Toolkit (Repast) (http://repast.sourceforge.net), a free, Java-based, open-source agent-based modeling environment (North et al., 2006). The model source code and documentation is available in the OpenABM models library (http://www.openabm.org/model/3872/version/1/view).

3.2. Proposed validation framework

Fig. 2 presents the validation framework we implemented for the PM. The framework relies mostly on the two main streams described in Section 2: (a) the conceptual validation of model components and processes and (b) the empirical validation. The conceptual validation involved a set of strategies aimed at ensuring the inclusion and realistic characterization of all relevant process. Interactions with stakeholders and domain experts supported several strategies in this stream. The empirical validation started later, after a first functional version of the model was subjected to a careful verification process. This stream involved a set of simulations aimed at comparing model outcomes with observed data and to identifying the need to adjust parameter values or include additional process. Note that although the two different validation streams are separated for the sake of presentation, there are multiple feedbacks between them. The next sections describe the strategies adopted as part of each stream and the main results obtained.

3.3. Conceptual validation

3.3.1. Approach for conceptual validation

The conceptual validation of the PM started in parallel with the design of the model. We adopted several design approaches that had the additional advantage of contributing to the validation of model components and processes. Following POM (Grimm et al., 2005), our model design – the definition of relevant variables and processes – was directed by the observed patterns that the model sought to explain, such as the concentration of farm ownership and soybean expansion (Fig. 2 – box 1). The observed patterns had a prominent role in the identification of necessary sub-models. For instance, the inclusion of the Update of Cropped Area sub-model (Fig. 1) corresponded to our interest in simulating the trajectories of the number and size of active farmers, as well as land tenure.

The design of each model component started with a review of the relevant literature and a simple initial design (Fig. 2 – boxes 2–4). We can distinguish two types of publications that contributed to the design of model components: (a) literature describing the theoretical basis of a relevant process or behavior and (b) documentation of other agent-based agricultural models with purposes very similar to ours. Specific examples of the first type of publication are articles by Lant (1992) and Diecidue and van de Ven (2008) that guided our design of the endogenous adjustment of an agents' aspiration level. Examples of the second type of publication are Polhill et al. (2010)'s FEARLUS paper, Happe et al. (2004)'s AgriPoliS paper, and Freeman et al. (2009)'s model of the Canadian Prairies. The design of several PM processes was built on these previously published models (see Table 1 in Bert et al., 2011) – an approach consistent with the TAPAS concept. The earliest result of our modeling effort was the structural design of the model and a simple initial design for each sub-model.

A highlight of our model development process has been the sustained participation of domain experts – members and technical staff from the Asociación Argentina de Consorcios Regionales de Experimentación Agrícola (AACREA), a collaborating farmers' organization (Orlove et al., 2011). The initial design of each PM sub-model was discussed in small workshops with three to five AACREA experts. All of the experts were technical advisors, while two of them also were farmers themselves. As we were designing each sub-model progressively, we held regular meetings with experts. During these interactions, model processes or components and underlying assumptions were presented, criticized, and discussed. Occasionally, the model design, main assumptions and preliminary results were presented during monthly meetings of project leaders for all ongoing AACREA research projects, a group that included over 20 experts. This process corresponds to the participation of independent subject matter experts recommended by Macal and North (2005). As a consequence of these interactions, in some cases it was necessary to redesign or modify the proposed components (Fig. 2 – box 5). The interaction with experts was not only useful to check the correctness and realism of the sub-models' initial design, but also to define specific processes, and in some cases parameter values involved in the various sub-models. A clear example of this was the parameterization of functions representing economies of scale, embedded in the Economic Calculations sub-module (Fig. 1).

3.3.2. Main results from conceptual validation

Following effective design principles and involving stakeholders from the beginning of the model design process produced positive feedback from the stakeholders. From the early stages, they felt that the PM included the essential structural and behavioral components, as well as a realistic characterization of important initial conditions and values for several model parameters. Additional evidence of the benefits of our approach is the fact that even the initial and very simplified set of simulations presented and discussed in Bert et al. (2011) produced very reasonable outcomes. These early simulations – even before any calibration – successfully reproduced the direction of the main structural and land tenure changes observed between 1988 and 2007. Additionally, the early simulations helped identify likely drivers for and provide plausible explanations of the dynamics of changes observed in the Pampas.

The initial results showed that the structural and land tenure changes in the Pampas seem to be largely driven by the long-run economic viability of individual farmers which, in turn, depends on the area they crop. Farmers cropping small areas are economically unviable in the long run and eventually must lease out their land to farmers with greater capital. This process leads to a "concentration of production" among fewer agents, and an increase in the area operated by tenants, as exiting farmers seldom sell their land but instead rent it out. In fact, the drivers identified from these simplified simulations were consistent with those identified by independent field studies: the disappearance of smaller farmers given their economic unviability is reported for the region by Cloquell et al. (2005) and Gallacher (2009) based on empirical data.

[1] The set may also include alternative agronomic management approaches for each activity (e.g., multiple ways to grow soybeans). However, in this manuscript we consider the single most common agronomic management approach for each activity.

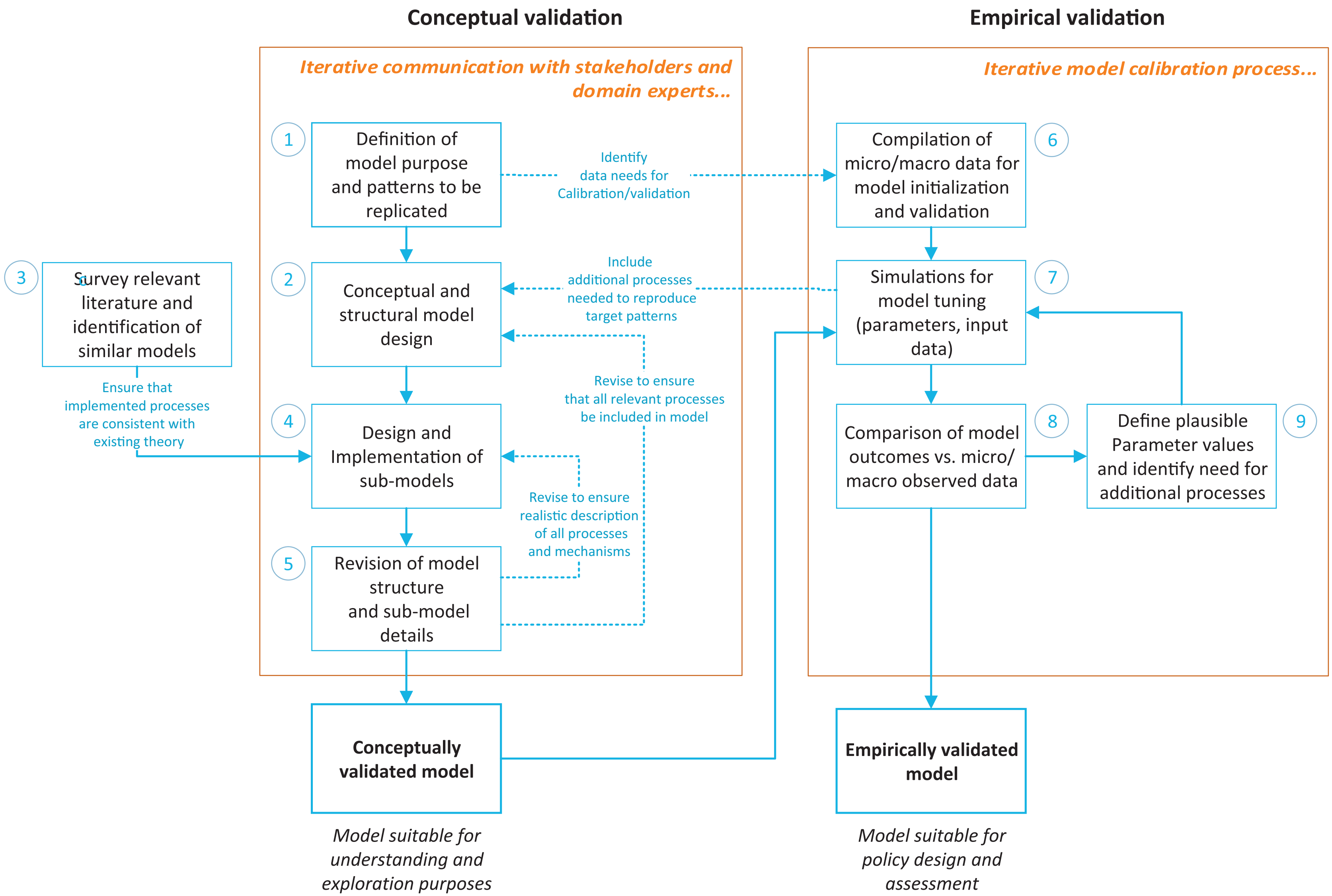

Fig. 2. Validation framework implemented for the validation of the Pampas Model.

In relation to land use, early simulations showed an increase of soybean area, linked to the higher profitability of this crop in recent years. Despite the stylized nature of early simulations, all emerging patterns were highly consistent with observed changes in the Pampas. Early results thus fulfilled one of the model validation criteria proposed by Gilbert (2008), which is the ability to replicate macro configurations that we wish to explain.

3.4. Empirical validation

3.4.1. Approach for empirical validation

The early ability of the PM to reproduce observed trends was very encouraging. However, we were interested in complementing the conceptual validation of model components with an empirical validation involving comparisons of simulated output and historical data. That is, we intended to assess not only if the model reproduced the main trends of structural and land use changes, but also the magnitude of such changes. Despite the potential pitfalls associated with the empirical validation of ABMs, any attempt in this direction has the potential to strengthen a model's legitimacy.

Our empirical validation focused on three factors. First, we wanted to assess the extent to which the model was able to reproduce reality. Second, we aimed to assess the model's sensitivity to a set of uncertain initial conditions and input variables. Third, we sought to identify the need for additional mechanisms not included in initial simple runs. As proposed by Topping et al. (2012), we used observed patterns to test, calibrate and further develop the PM.

The empirical validation of the PM involved multiple simulations that included many of the steps suggested by Windrum et al. (2007) for empirical validation of ABMs (Fig. 2): (a) initialization data and trajectories of input variables were defined as realistically as possible using micro/macro empirical data (Fig. 2 – box 6), (b) an initial realistic scenario was run (Fig. 2 – box 7), (c) simulated results were compared with observed patterns (Fig. 2 – box 8), (d) for those cases in which differences between simulated and observed patterns were detected, alternative hypotheses addressing the mismatches were proposed, and (e) according to these hypotheses, new scenarios were run assuming plausible realistic changes and/or adjustments in scenario attributes (Fig. 2 – boxes 7, 9). In the following sections we describe the simulations performed and changes introduced in the model that resulted from the empirical validation.

3.4.1.1. Initialization and input data. Initialization data and trajectories of inputs required by simulations were compiled from multiple sources. There are only two National Agricultural Censuses (NACs) available in Argentina for the period simulated: the 1988 (NAC88) and 2002 (NAC02) censuses. We started simulations in 1988 because NAC88 provided most of the information needed to initialize the model. Even though simulations were run through 2007, we used NAC02 data as a reference waypoint to compare simulated and observed patterns. We also collected information from agricultural statistics from the Ministerio de Agricultura, Ganadería y Pesca de la Nación Argentina (MAGyP) and trade magazines. Specific use of these data is described below.

Model initialization procedures were designed to ensure that (i) the distribution of simulated farm sizes, (ii) the number of farms, farmers and total area operated by each farmer, (iii) land use, and (iv) the proportion of area operated by owners and tenants were all consistent with data from the 1988 Census. The distribution of individual farm sizes had to be estimated indirectly, because the NAC88 does not list these values; instead, it includes only the *total area* and *number* of farms operated by each farmer. Thus we used cadastral information available only for part (about 30%) of the area to extrapolate the distribution of farm sizes for the entire region. Data from NAC88 also were used to initialize the number of active farmers and the area operated by each agent (each farmer was assigned one or more owned and/or rented farms). Each plot in a farm was randomly assigned with an initial crop with a probability proportional to the area reported for each crop in the 1988 MAGyP statistics. The initialization of activities within each farm also respected the crop rotation preference assigned to the farm operator: for example, if the agent was a "strict rotator," a maximum of 1/3 of the land was possible for each of the three activities considered. Table 1 provides details about initial values of main relevant model variables.

The inputs required to calculate farm profits were: (a) costs of inputs (e.g., seeds, agrochemicals) for all modeled agricultural activities, (b) commodity prices and (c) yields of all activities. The PM has modules to compute the Gross Margin (GM) based on these inputs (Fig. 1). Alternatively, GM for each activity can be provided as

Table 1
Summary of initial (1988) values assigned to main model variables. These initial conditions were held constant across all scenarios presented in this paper. Values were determined based on data from National Agricultural Census 1988 (NAC1988) and records from the Ministerio de Agricultura, Ganadería y Pesca de la Nación Argentina (MAGyP).

Variable	Details	Value	Source
Number of farms		10,037	NAC88
Total area (hectares)		929,762	NAC88
Min farm size (hectares)		7.5	NAC88 and cadaster available
Max farm size (hectares)		3291	
Number of active farmers		4439	NAC88
Number (proportion) of farmers by category of extension (hectares)	<25	215 (4.8%)	NAC88
	25.1–50	893 (20.1%)	
	50.1–100	1144 (25.8%)	
	100.1–200	983 (22.1%)	
	200.1–500	822 (18.5%)	
	500.1–1000	243 (5.5%)	
	1000.1–1500	76 (1.7%)	
	1500.1–2000	27 (0.61%)	
	2000.1–2500	20 (0.45%)	
	2500.1–3500	11 (0.25%)	
	3500.1–5000	2 (0.05%)	
	>5000	3 (0.07%)	
Total area (proportion) operated by	Owners	528,063 (62.6%)	NAC88
	Tenants	347,699 (37.4%)	
Total area (proportion) occupied by	Soybean	395,853 (42.5%)	NAC88 and MAGyP
	Maize	244,210 (26.3%)	
	Wheat	289,699 (31.2%)	

Table 2
Description of model mechanisms and their parameter values, initialization values and input data tested during the calibration and validation process.

Simulation group	Model detail type	Model detail name	Tested options
Group 1: Structure and land tenure	Initialization	Distribution of Initial WC of farmers	• Homogeneous ($500 for owners, $1000 for tenants) • Uniform ($250–1000 for owners, $500–2000 for tenants) • Normally distributed: mean $500 and standard deviation $100 for owners; mean $1000 and standard deviation $250 for tenants
	Mechanisms and parameters	Minimum progress rate	• Off • On (rate equal to 5%)
		Off-farm income	• Off • On: – $18 K for 25% of all farmers – $18 K for 50% of all farmers – $18 K for 50% of farmers operating < 200 ha
		Retirement	• No retirement • Retirement activated – 1.0% per year – 0.5% per year – 1.5% per year
Group 2: land use	Initialization	Rotator type	• Owners: 50% "flexible" and 50% "very flexible", Tenants: "non-rotators" • Owners: "non-rotators", Tenants: "non-rotators'
	Mechanisms and parameters	Search triggering mechanism (STM)	• "N out of M" • Random • 50% N out of M, 50% Random
		Land use selection mechanism (LUSM)	• Maximization of Cumulative Prospect Theory (CPT) value • Maximization of Expected Utility (EU) • 50% CPT maximizers, 50% Imitators
		N and M values (for "N out of M" STM)	• $N=2$ and $M=3$ • $N=1$ and $M=2$ • $N=1$ and $M=3$
		Probability of search being triggered (for "Random" STM)	• $P=1.0$ • $P=0.5$
		Alpha and Lambda parameters (for CPT LUSM)	• Published Alpha and Lambda values (0.88 and 2.25) • Alpha and Lambda values from AACREA surveys
		Optimization window (for CPT and EU LUSMs)	• 1 year • 3 years • 5 years
	Historical data sources	Gross margin of agricultural activities	• Agromercado • Márgenes Agropecuarios • Ministerio de Agricultura, Ganadería y Pesca (MAGyP)

input data. Because it is difficult to get reliable historical series for input types and amounts used and their historical costs – needed by economic calculations within the model – it was more realistic to provide GM data as input. For this reason, we used published series (1980 to present) of GMs for different agricultural activities.

Other required inputs are series of expected and actual status of contextual factors that influence the dynamic formation of an aspiration level. These series were defined based on limited available information about commodity prices, input costs, and rainfall.[2] There was no empirical information available to initialize some required variables (e.g., the agents' working capital or their land use selection mechanism). In such cases, we tested the sensitivity of simulated outcomes to a range of plausible values during the calibration process described below.

3.4.1.2. Organization of simulation experiments. All simulations were performed with the same version of the PM introduced in Bert et al. (2011) plus the enhancements included in the "Update of Cropped Area" sub-model (details in Appendix A). Other necessary model adjustments were identified during the validation and calibration processes and will be described below.

We simulated several different scenarios encompassing the period 1988–2007. Each scenario (run) was characterized by a specific set of model mechanisms and parameters; initial conditions; and trajectories of input variables. Many simulation inputs (e.g., number of farms, farm size distribution, etc.) remained unchanged across all scenarios. Results from earlier simulations (Bert et al., 2011) had suggested that the various historical patterns studied – although highly related – seemed to be triggered by different drivers. For this reason, we designed two separate and consecutive groups of simulations: Group 1 included 25 scenarios aimed at validating and calibrating the model in relation to structural and land tenure changes; Group 2 involved 28 scenarios intended to validate and calibrate the model from the point of view of land use changes. Table 2 shows the variables and options tested in each group. The options tested in each scenario group encompassed: (a) alternative realistic values for uncertain initial conditions (e.g., working capital of farmers), (b) alternative available trajectories for input data (e.g., gross margins from different available sources), (c) different assignment of possible mechanisms or parameter values among agents (e.g., land use selection mechanisms) and (d) activation or deactivation of overall mechanisms (e.g., farmer retirement). The scenarios varied one, and occasionally two, variables at a time, keeping all the rest at nominal values. However, as model evaluation progressed,

[2] Our model considers three main context factors: climate, output prices and input costs (Fig. 1). The expected and actual statuses of these factors – for each cropping cycle – are categorized as favorable (F), normal (N) and unfavorable (U). The expected and actual statuses assumed in these simulations were as follows: *Climate:* The expected status was always N. The actual status was F, N or U according to total rainfall in the period September to February. *Output prices:* The expected status for cycle time t was F, N or U according to future prices (for t) in $t-1$. The actual status was F, N or U depending on output prices in t. In both cases, the status was defined individually for each activity and then a modal status was computed. *Input costs:* The expected status was F, N or U according to available, but incomplete, series of fixed direct costs. The status was defined individually for each activity and then a modal status was computed. As the temporal variability of input prices is low, the actual status was equal to the expected status. A similar concept of expected and actual context was used by Kellermann et al. (2008).

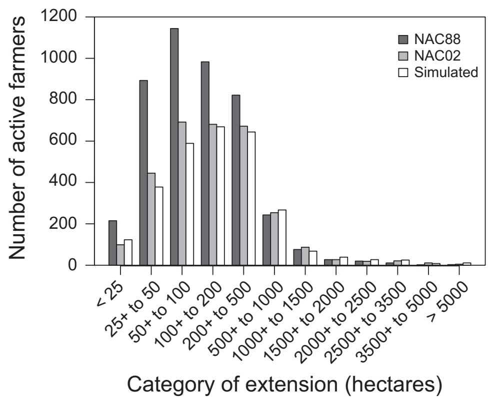

Fig. 3. Number of farmers by category from: (i) 1988 National Agricultural Census ("NAC88"; dark gray bars), (ii) 2002 National Agricultural Census ("NAC02"; light gray bars) and (iii) simulations of PM for cropping cycle 2001/02 ("simulated"; white bars).

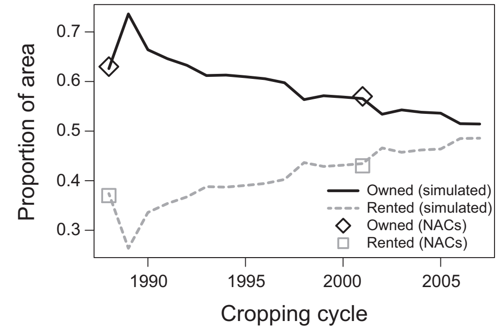

Fig. 4. Proportion of total area operated by owners and tenants: (i) proportion of owned area simulated by PM ("Owned (simulated)"; black line), (ii) proportion of owned area from 1988 and 2002 National Agricultural Censuses ("Owned (NACs)"; black rhombi), (iii) proportion of rental area simulated by PM ("rented (simulated)"; gray dashed line) and (iv) proportion of rented area from 1988 and 2002 National Agricultural Censuses ("rented (NACs)"; gray squares).

the scenarios included adjustments in values of variables defined in preceding scenarios.

3.4.2. Main results from empirical validation

3.4.2.1. Observed and simulated structural and land tenure patterns. All Group 1 scenarios reproduced qualitatively the major structural trends observed: (a) decrease in the number of active farmers, in particular those operating smaller areas, (b) increase in the average area operated by active farmers (i.e., concentration of production), and (c) increase in both the number of farms and total area operated by tenants. The quantitative agreement between simulated and historical data, however, was uneven for the various indices. In the period 1988–2002, the actual number of active farmers decreased 32.1%, while different model scenarios simulated decreases between 20.5 and 49.9% (median: 35.8%). The median area cropped by a farmer increased 30% in the simulated region the same period (from 100 to 130 ha), whereas the model simulated increases from 34 to 141% (median: 64%). That is, some scenarios greatly overestimated the concentration of land. Finally, the number of farms operated by owners decreased 22.6%, whereas simulated decreases ranged from 13 to 38% (median 25.9%). Unlike results for the *number of farms*, the model was initially unable to reproduce the qualitative trend in the *proportion of area* operated by owners. This finding will be discussed below. While census data showed a clear decrease in the area operated by owners (7.9%), simulation results were ambiguous: some of the scenarios produced increases (up to 5.8%) while others showed decreases (up to 10.1%).

Although the first few scenarios of Group 1 mimicked the *direction* of structural and tenure changes, detailed calibration was required to reproduce the *magnitude* of such changes. Simulated results from successive Group 1 scenarios got closer to historical values reported in NAC02. The latest scenarios reproduced the magnitude of the disappearance of small farmers (<200 ha) and the corresponding increase in the number of large farmers reported in NACs (Fig. 3). These simulations also reproduced well the changes in the distribution of total area operated by each agent (Table 3).

Table 3
Quintiles of total operated area by farmer for: (i) 1988 National Agricultural Census ("NAC88"), (ii) 2002 National Agricultural Census ("NAC02") and (iii) simulations of PM for cropping cycle 2001/02 for a post-calibration scenario ("simulated").

Quintile	NAC 1988	NAC 2002	Simulated
5	26	29	27
25	51	62	67
50	100	130	145
75	217	304	324
90	714	1081	1217

Although the simulated distribution of area operated by each agent in 2002 was statistically different from that reported in NAC02 (Kolmogorov–Smirnov test, $p = 0.04$), earlier calibration scenarios had shown much larger differences (e.g., $p = 2.2 \times 10^{-16}$). Finally, the calibrated model reproduced the magnitude of land tenure changes (Fig. 4): with the exception of early instability, the proportion of area operated by tenants (owners) gradually increased (decreased) throughout the simulations. In 2002, the proportion of area rented was very similar to the NAC value (45%). By the end of simulations it had reached almost 50%, a number consistent with recent reports (Reboratti, 2010).

The calibration process allowed us to identify and add or activate model mechanisms initially deemed unimportant. Without these mechanisms, it was not possible to reproduce closely the magnitude of observed changes described in the precedent paragraph. For instance, in the first few scenarios of Group 1, 70% of simulated farmers cropping <200 ha had disappeared by 2002. The decrease was even more dramatic for farmers operating <50 ha: 98% of these agents had exited production by 2002. In contrast, census data show that the actual decrease in the number of smaller farmers was not as pronounced. Only 40% of small farmers (as opposed to the simulated 70%) had exited production by 2002 (Gallacher, 2009).

The difference between observed and simulated survival rates of small farmers could not be explained without assuming that some of these agents had off-farm sources of income (e.g., providing services to other farmers, or jobs or businesses in nearby towns). Previous studies in several places, including the Pampas, highlighted the crucial importance of off-farm income for the economic viability of small farmers (Cloquell et al., 2005; Gallacher, 2009; Goddard et al., 1993; Zimmermann and Heckelei, 2012).

As in other ABMs of agriculture (Freeman et al., 2009; Happe et al., 2004), off-farm income was implemented beginning with early versions of the PM. Nonetheless, it was not activated during the initial simulations. In the simulations described here, we had to assign off-farm incomes to small farmers in order to avoid overestimating the exit rates for these farmers. We explored various plausible values for both (i) annual off-farm income level and (ii) the proportion of farmers receiving it (Table 2). Results shown in Fig. 3 assumed that 50% of farmers initially operating <200 ha received an annual off-farm income of $18,000 (i.e., they do not need any farming income to cover household expenses).

As mentioned above, early calibration scenarios did not fully reproduce the trend and magnitude of land tenure changes. In these simulations, most farmers leaving active status, and thus renting out their land to others, cropped small areas. In other words, economically viable medium and large farms were predominantly operated by their owners, who also rented several small farms. Consequently, the number of farms operated by tenants was high, but these farms only accounted for a small proportion of total area. These results are different than the observed data, not only in relation to the proportion of rented area, but also because NAC02 shows several large farms (e.g., 45.3 and 37.9% of farms larger than 200 and 500 ha respectively) that are operated by tenants. In contrast, the proportion of farms run by tenants in early calibration simulations was much lower: 22.3 and 7.7% of farms larger than 200 and 500 ha respectively.

To address the underestimation of the area operated by farmers, during calibration we introduced an additional mechanism associated with the agentsí life cycle: the "forced exit" or retirement of agents. With this mechanism, a number of randomly selected agents exit production every cycle, regardless of their financial status or prior economic progress. A similar process was used by Freeman et al. (2009) in their ABM of the Canadian Prairies. This mechanism attempts to capture the empirical observation that once a farmer reaches retirement age, sometimes their heirs do not wish to continue running the family farm and therefore rent it out.

In scenarios where the "retirement" mechanism was activated (e.g., Fig. 3), the model fit was enhanced. The proportion of total area operated by tenants increased significantly (from 32.5% in 1988 to 42.7% in 2001). The proportion of agents who retire each year is a parameter of this mechanism. Multiple plausible values were explored (Table 2). Results shown in Fig. 4 are based on a retirement rate of 1% per year, a realistic value based on data from Argentina's 2001 Population Census.

3.4.2.2. Observed and simulated land use patterns. The simulated results discussed in this section involve land use selection mechanisms tied only to the maximization of an economic goal (e.g., the expected utility of changes in total wealth, or the Prospect Theory value of gross margins relative to a reference point). Consequently, simulated land use was extremely sensitive to the relative profitability of modeled agricultural activities. Differences in profitability among crops were described through time series of gross margins (GMs) for full-cycle soybean, maize, and wheat-soybean double crop. Deflated historical GM series were compiled from three different sources: two trade magazines (Agromercado and Márgenes Agropecuarios) and the official MAGyP statistics (Table 2). The GM series were generally similar for the three data sources, but differences were present in some years.[3]

Historical MAGyP records show that soybean dominated maize and wheat during the entire simulated period, particularly after the mid-1990s (Fig. 5). Nevertheless, only the simulations performed with the Agromercado GMs reproduced the sustained predominance of soybean. Results from Ordinal Pattern Analysis (OPA) (Thorngate and Edmonds, 2013) showed that these simulations also captured the increase in the rate of soybean expansion in the mid 1990s (Table 4). In contrast, simulations based on GM series from Márgenes Agropecuarios and MAGyP led to comparable proportions of all crops, without marked temporal changes throughout the simulated period. That is, these historical sources did not allow us to reproduce the trend toward increasing soybean acreage (Fig. 5 and Table 4).

Differences among GM series introduced variability in the relative profitability of crops that created differences in simulated land uses as shown in Fig. 5. For instance, from 2000 to 2007 the soybean-to-maize GM ratio varied between 1.11 and 3.31 in Agromercado

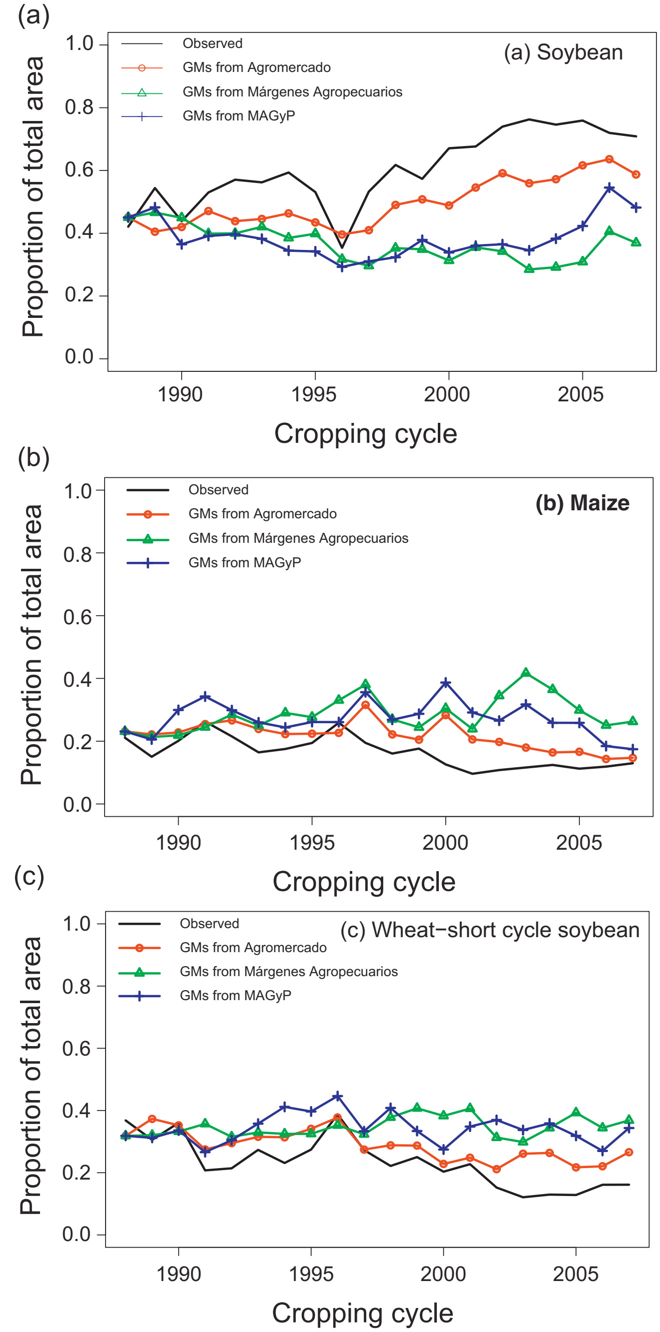

Fig. 5. Proportion of total area assigned to (a) soybean, (b) maize and (c) wheat-soybean: (i) observed records from the Ministerio de Agricultura, Ganadería y Pesca (MAGyP) (black line without symbols), (ii) simulated by PM using the series of Gross Margins (GM) from Agromercado magazine as input (red line and circles), (iii) simulated by PM using the series of GM from Márgenes Agropecuarios magazine as input (green line and triangles) and (iv) simulated by PM using the series of GM from MAGyP as input (blue line and crosses). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

data, whereas the same quantity varied between 0.72 and 1.72 in Márgenes Agropecuarios data. As result, the 2000 to 2007 average proportion of simulated soybean area was 33.4% and 57.5% using GM data from Márgenes Agropecuarios and Agromercado, respectively. The corresponding average proportion of maize area was 31.0% and 18.6%.

Although the PM reproduced the *trend* toward increasing soybean area using GMs from Agromercado, none of the available sources of economic data allowed us to reproduce the full

[3] See Table B1 – Appendix B.

Table 4
Ordinal fit between observed and simulated proportion of area assigned to soybean, maize and wheat/soybean using alternative sources of gross margins including the probability of a match (POM), the index of observed fit (IOF), the probability of matches higher or equal obtained matches (Prob), and the root mean square error (RMSE). Observed data is from Ministerio de Agricultura, Ganadería y Pesca records.

Activity	GM source	POM	IOF	Prob	RMSE
	Agromercado	0.892	+0.785	0	0.123
Soybean	Márgenes Agropecuarios	0.215	−0.570	1	0.278
	MAGyP	0.551	+0.101	0.307	0.246
	Agromercado	0.396	−0.208	0.827	0.067
Maize	Márgenes Agropecuarios	0.708	+0.417	0.045	0.144
	MAGyP	0.542	+0.083	0.384	0.124
	Agromercado	0.667	+0.333	0.116	0.071
Wheat	Márgenes Agropecuarios	0.762	+0.524	0.032	0.144
	MAGyP	0.714	+0.429	0.054	0.135

magnitude of the soybean increase (see Root Mean Square Error[4] in Table 4). Historical data showed that the proportion of soybean area was >70% after 2001, whereas the simulations only reached maximum values of 63.6%. Correspondingly, the PM over-estimated the area allocated to maize and the wheat/short cycle soybean double crop (particularly after 2002).

The underestimation of the magnitude of soybean area may be the result of several plausible causes. One possibility is that the PM is not considering all mechanisms or variables relevant to land use selection. The current land use selection considers only the GM of each activity. Nevertheless, other criteria – such as the relative costs of different crops – also may be highly relevant to choosing land use. Some of these costs are incurred before the crop is sold, and must be covered by a farmer's working capital. We note that in the current PM we assume that farmers have the capital to afford any activity; this assumption may not be entirely realistic.

Production costs may vary significantly among activities. For example, soybean production costs have decreased considerably because no-till planting and herbicide-tolerant genotypes require less mechanical labor and fuel (Qaim and Traxler, 2005; Reboratti, 2010). As a result, in recent years (2002–2007) the median direct costs of maize were about 2.6 times higher than soybean costs.[5] This marked difference in out-of-pocket costs, however, was not fully reflected in the final profitability of each activity. For instance, in Agromercado median soybean GM in the period 2000–2007 was 1.6 times higher than maize GM. Similarly, Márgenes Agropecuarios median soybean GM in the same period was 0.95 times higher. Preliminary experimentation with multi-objective land use selection – in which profits and costs are simultaneously considered – shows that consideration of costs leads to higher proportions of soybeans. In other words, given similar relative profits, farmers may prefer to crop more hectares of the crop requiring a lower initial investment, in this case soybeans.

Another possible reason behind the underestimation of soybean expansion is that the current PM assumes that total cropland area does not change during the simulation. In reality, there was an expansion of agriculture toward marginal areas formerly occupied by pastures and natural grasslands (Paruelo et al., 2005). This process was not as marked in Northern Buenos Aires: this region of excellent climate and soils already had a long agricultural tradition, thus total cropped area increased only 27.9% since 1988. When new lands – usually of lower quality – are occupied by agriculture, soybean is the crop of choice because of its ecological adaptability and simplicity of management (Paruelo et al., 2005). As a result, the

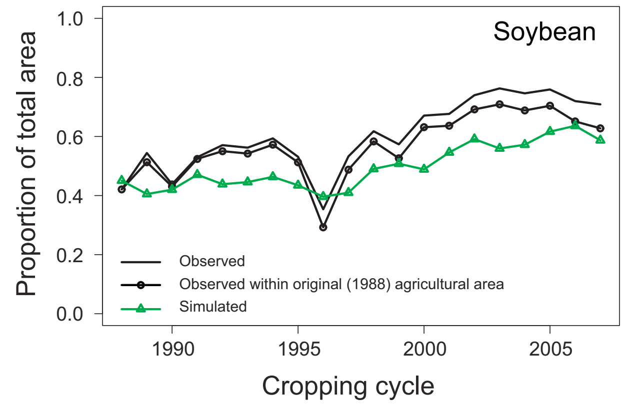

Fig. 6. Proportion of area with soybean: (i) from records of MAGyP (black line without symbols), (ii) from records of MAGyP, but assuming that the entire area converted to agriculture was planted with soybean and removing this area from calculations of soybean proportion (black line and circles) and (iii) from PM simulations using Agromercado's GM (green line and triangles). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

growing dominance of soybean could be associated not only with changes in crop proportions within the traditional agricultural area, but also to a preference for soybean in areas recently converted to agriculture.

If we assumed only hypothetically that the entire area converted to agriculture was planted with soybean, and removed this area from the calculation of observed soybean proportion[6] (that is, if we froze the agricultural area to its extent at the beginning of simulations), the increase in soybean proportion would be lower. Nevertheless, even with this assumption the PM would have been unable to reproduce the full magnitude of soybean expansion (Fig. 6). These results suggest the need to consider additional or alternative land use selection mechanisms in order to quantitatively reproduce the observed patterns. Future versions of the model will explore these issues.

Finally, as the implementation of human decision-making processes is one of the main strengths of ABMs, the agent attributes and behavioral functions that represent these processes require appropriate description. Li (2012) and Smajgl et al. (2011) review methods used to characterize human decision-making in ABMs. In many cases, there is no empirical information available that can be used to assign mechanisms and parameter values to agents, or to define the proportion of agents relying on different candidate mechanisms. For this reason, during the calibration we explored briefly the sensitivity of outcomes to the main model mechanisms, the associated parameters, and agent attributes related to land use decision-making. As detailed in Table 2, the agent attributes were (a) the agent's rotator type (i.e., the agent's willingness to rotate crops), and (b) the Search Triggering (ST) and (c) Land Use Selection (LUS) mechanisms.

Simulated land use did not change significantly in response to the agents' crop rotation preferences (Fig. 7a). Conversely, the ST mechanism introduced larger differences in simulated outcomes (Fig. 7b). The "N out of M" ST mechanism[7] yielded very stable land uses, whereas the "Random" mechanism produced much short-term variability. The actual land use change patterns seem to be in between these extremes. The results discussed above assumed "*N* out of *M*" for half of farmers and "Random" for the

[4] We we computed RMSE as a complement to OPA since OPA indicates the topological fit between observed and simulated outputs but does not consider their closeness.

[5] 330 $ ha-1 vs. 130 $ ha-1, respectively. Costs usually show low inter-annual variability.

[6] Records from MAGyP do not allow us to separate traditional and newly cropped areas.

[7] Search is triggered if the farmer has been "unsatisfied" with *N* economic outcomes in the *M* most recent cycles.

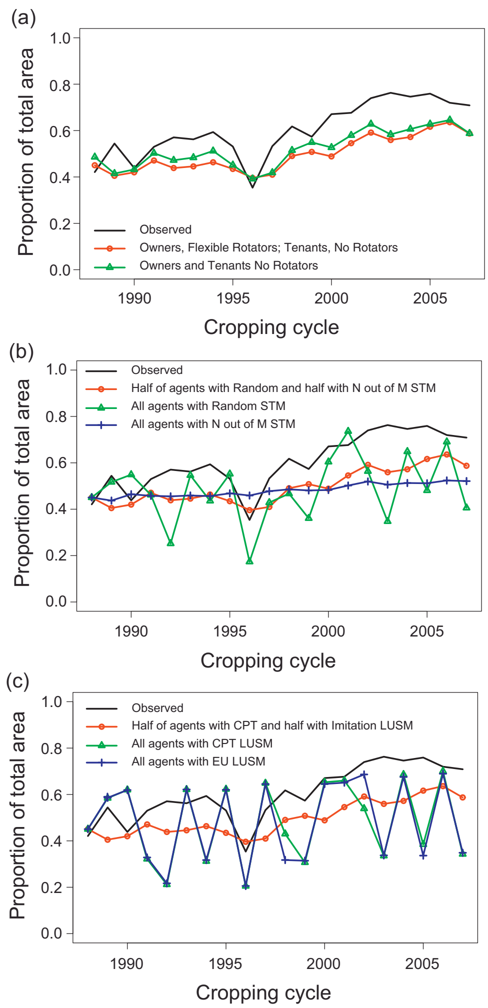

Fig. 7. Proportion of soybean for different simulated scenarios: (a) scenarios aimed to assess impacts of farmers' rotation type: (i) all owners are flexible rotators (i.e., any activity cannot cover more than 50% of farm area) and all tenants are no rotators (a single activity can cover up to 100% of farm area) (red line and circles) and (ii) owners and tenants are No rotators (green line and triangles). (b) Scenarios aimed to assess sensitivity to farmers' Search Triggering Mechanisms (STM): (i) half of farmers are assigned the Random STM and the other half the "N out of M" STM (red line and circles), (ii) all farmers are assigned the Random STM (green line and triangles) and (iii) all farmers are assigned the "N out of M" STM (blue line and crosses). (c) Scenarios aimed to assess sensitivity to farmers' Land Use Selection Mechanisms (LUSM): (i) half of farmers are assigned the Random Cumulative Prospect Theory (CPT) LUSM and the other half the Imitation LUSM (red line and circles), (b) all farmers are assigned the CPT LUSM (green line and triangles) and (c) all farmers are assigned the Expected Utility (EU) LUSM (blue line and crosses). All figures include the observed proportion of soybean from MAGyP (black line without symbols). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

other half. The LUS mechanism also introduced differences in simulated outcomes (Fig. 7c). When all farmers maximize an objective function – Cumulative Prospect Theory (CPT) or expected utility – there is significant inter-annual variability in the area of each activity. Instead, land use selection via imitation produces much smoother temporal fluctuations. Again, observed patterns suggest an intermediate scale of variability, which we achieve by combining land use selection mechanisms (half of the agents maximize CPT and the other half are "imitators"). Although we cannot be completely sure about the types and proportions of ST and LUS mechanisms without fieldwork, these initial sensitivity analyses allowed us to identify, and discard, settings that lead to completely unrealistic outcomes or dynamics (i.e., settings that invalidate the model; Macal and North, 2005).

4. Lessons from our validation experience

Many valuable results and lessons emerged from the PM validation process. Some of our findings may have general utility for the ABM community, while other findings are relevant for future uses of our model. The following sections discuss both groups of results.

4.1. Lessons from our validation process

We believe that our PM validation efforts yielded a set of potentially valuable lessons for others working on agent-based models. We stress here the main four lessons learned:

1. *Address validation from both "conceptual" and "empirical" viewpoints.* We recommend organizing all validation efforts into two complementary streams: (a) validation of model components and processes ("conceptual validation") and (b) validation of model outcomes ("empirical validation"). The validation of model components and processes must start from the very beginning of model development. This stream mainly seeks to ensure realism in model structure and processes. Conceptual validation may rely on multiple strategies that guide model design and implementation (Fig. 2) including (a) spending as much time as needed defining model purpose and the patterns to be replicated, (b) survey the relevant literature to identify similar models and the processes they include, and (c) involve stakeholders in model design. This list is not exhaustive. Only after reaching an initial functional version of the model, we recommend validation efforts involving the comparison of simulated outcomes against empirical field data. The empirical validation stream seeks mainly to assess the model's ability to reproduce observed patterns, although it can actually achieve much more than that, as discussed below.
2. *Start off on the right foot: validate individual model processes and components.* Our experience clearly showed the valuable results that careful conceptual validation could yield. From the earliest stages, the PM included the necessary structural and behavioral components as well as realistic characterizations of important initial conditions and parameters. The best evidence of the benefit of such approach was the reasonableness of early PM results (Bert et al., 2011). Starting with early simulations – even before any calibration – the PM successfully reproduced the dynamics of the main structural and land tenure changes recently observed in the Pampas. Strategies useful for conceptual validation – mainly interactions with stakeholders – are not only intended to determine the validity of your design, but also to the reveal processes and parameters for which information is not available.
3. *Do everything possible to validate model results against observed data.* Despite the difficulties in traditional validation of agent-based models, we strongly recommend that – whenever possible – efforts be made to perform an empirical validation. Unfortunately there are not many examples of empirical validation of agent-based models; notable exceptions include Freeman et al. (2009) and Damgaard et al. (2009). Simulations with outputs designed to be compared with observed patterns allow not only empirical falsification but also to (a) define plausible spaces of parameters values[8] and (b) identify processes that may have been ignored or deemed unimportant during model design (Fig. 2 – box 9). Topping et al. (2012), using what they called Post Hoc POM, showed that real world patterns may drive model tuning and testing. Our experience reinforces this finding: even having adopted good modeling practices for model design and

[8] This is critical as it is common for many parameters in models to be uncertain.

development, the observed patterns and comparisons with simulations led to a tuning and further development of the model. The necessary inclusion of off-farm income is very illustrative. It was considered in early versions of the PM, as it was included in similar models (e.g., Agripolis), but was initially "turned off". Simulations subsequently showed that off-farm income was critical for the survival of smaller farmers. The need for this mechanism did not emerge during interactions with stakeholders, as AACREA members tend to farm land areas that are above average, and thus need not depend on additional income sources (this omission could be considered as "biased design").

4. *Do not discard the model if empirical validation of outcomes is not possible.* We have previously recommended undertaking an empirical validation, but we acknowledge that this is not always possible or necessary for a model to be valid. As we describe in our framework (Fig. 2), we distinguish two validation levels associated to our two separate validation streams that enable different uses of the model. If only a conceptual validation is possible, the resulting model still may be useful to describe, understand or explore the system being studied. However, if the model is intended for policy design and assessment, our experience showed that some kind of empirical validation is critical. In our case, although the strategies for conceptual validation led to a model that realistically reproduced the direction of main patterns of interest, empirical validation was essential to reproduce the *magnitude* of such patterns. Given the adjustments of the PM that emerged from the empirical validation process, we would not have had confidence in the pre-empirical validated version of the model for its use in policy assessment (e.g., how many farmers would benefit if a given policy is implemented?). We are aware that initial versions of a model may be useful to understand the dynamics of the system and to envision plausible policies, but the quantification of policy impacts – one of the main advantages of agent-based models – cannot be reliably achieved without confirming that the model is able to reproduce real world patterns with sufficient accuracy.
5. *Confidence is gained step by step:* Our proposed validation framework involves multiple validation strategies, from early reviews of the model's structural design to the comparison of simulated outcomes against real world data. All these strategies informed the model formulation, thus contributing to make a better model. The strategies encompassed by the conceptual validation were essential to ensure a realistic model design. The review of relevant literature and similar models guided our design on the basis of well-understood and accepted concepts and theories. In turn, iterative communication with stakeholders led us to identify, specify and/or redefine model processes and rules, enhancing the model's level of realism (see specific examples in Section 3.3). The empirical validation process was essential to define model parameters values and identify additional processes needed to reproduce target patterns (see specific examples sin Section 3.4). This feedback from empirical validation to model design was an unexpected finding, as usually the empirical validation is focused on assessing the extent to which the model reproduces reality. No one strategy or test was determinant to accept the model as a valid tool for answering important questions. Instead, we gradually gained confidence in the model as each step of the validation framework was completed.

4.2. Implications of the validation process for uses of the Pampas Model

This manuscript focused on the validation of the PM, an agent-based model of agricultural systems in Argentina, and the lessons that can be extracted from this effort. Nevertheless, one should not lose sight of the fact that validation is undertaken for a purpose: to ensure that a model reflects appropriately the main behaviors of the target system. After completing the multiple validation steps described above, we are confident that the PM has achieved a reasonable level of realism. Indeed, the PM effectively reproduced both the trends and magnitude of real-world changes in the Pampas. Our evaluation process suggests that the PM can serve the purpose for which it was originally formulated (Rand and Rust, 2011), namely, to gain insights into the dynamics of recent structural and land use changes in agricultural systems of the Argentine Pampas. Moreover, we are confident that the PM can be used to explore future or non-observable scenarios.

Future use of the PM will be focused on exploring outcomes of alternative policies or the system's response to evolving scenarios (e.g., changes in climate conditions). Bert et al. (2011) found that structural and tenure changes in the Pampas were closely tied to the economic viability of farmers operating small land areas. The results presented here suggest also that the structural changes would be even more dramatic if a significant proportion of small farmers did not have supplementary off-farm income (e.g., provision of services, off-farm employment). Policies seeking to avoid the disappearance of smaller farmers and the concentration of production among fewer farmers may leverage these findings. For instance, as discussed by Bert et al. (2011), the provision of subsidies or tax breaks to smaller farmers during low-income years (e.g., years with adverse climate or crop prices) would not ensure the long-term economic viability of small farmers. Instead, encouraging small farmers to generate off-farm income by developing agriculturally related activities would allow them to stay in business.

Land use changes in the Pampas are strongly tied to the relative profitability of agricultural activities (Bert et al., 2011). However, results shown here showed that the PM was not fully able to reproduce the magnitude of land use changes using only relative gross margins. This result suggests that other attributes – such as the investment required by each agricultural activity – may be important for land use decisions. In fact, gross margins of soybeans were not much higher than those for maize during the last few years, whereas maize production costs were almost twice as high as soybean costs.

Because worries are growing about the increasing "soybean monoculture" (Viglizzo et al., 2011), the PM can be used to explore alternative policies to mitigate this trend. At least two alternative, and not mutually exclusive, policies may be envisioned to slow soybean monoculture and encourage ecologically-sound crop rotation: (a) to modify the relative profitability of different activities by adjusting the level of taxes (e.g., export taxes) applied to each activity; and (b) to modify the relative production costs of alternative activities by reducing the costs of specific inputs. Regarding the first option, the Government of Argentina already has set differential export tax levels: 35%, 23% and 20% for soybean, wheat and maize respectively. Regarding the cost of inputs policy, there have been attempts to decrease the costs of expensive inputs used mainly for maize and wheat (e.g., nitrogen fertilizer). So far, neither policy has been sufficient to discourage soybean expansion. The validated PM provides a virtual laboratory in which the impacts of these and other alternative policies could be explored in a realistic context that captures most of the system complexity.

Finally, as a result of the validation process we have identified some limitations on the use of the PM. One of the main limitations is associated with the availability of empirical data to determine model initialization values and settings. This is a frequent limitation in the domains in which ABMs are employed (Bharathy and Silverman, 2013). The lack of data is particularly important for the definition of agents' attributes (e.g., parameter values for decision-making mechanisms, parameter values for the aspiration level model, etc.). Field research is necessary to define more accurately the attributes of multiple agents. Our experience has also shown that the existence of alternative but inconsistent sources of data (e.g., sources of gross margin) may be a limitation in relation to data to inform model runs. Another significant limitation of the PM is that it does not consider livestock production systems. This is not a great concern for modeling historically agricultural areas (as Northern Buenos Aires, studied here), but we should consider cattle farming in order to use the PM in areas where agriculture has expanded recently, displacing livestock systems, and where livestock production remains an important land use. Further, although the current version of the model captures most of the observed land use changes, our results showed the need for testing new decision-making mechanisms beyond just comparing the gross margins of alternative activities. In summary, our model – as are most large-scale ABMs – is still a work in progress.

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Appendix A.

Two main processes of the "Update of Cropped Area" (Fig. 1) sub-model were updated in relation to the PM version presented in Bert et al. (2011). First, in the previous PM version land rental price (LRP) was exogenously defined and provided as an input variable. In contrast, in the new version we implemented LARMA, a *LAnd Rental MArket Model* with endogenous LRP formation (Bert et al., 2010). Second, in the earlier PM version we had assumed that farms were rented out only by owners who did not have sufficient WC to continue farming their land. We introduced two additional processes that could induce owners to rent out their land. First, owners who have sufficient WC on any given cycle may nevertheless be unhappy with their recent economic progress. If LRP is sufficiently high, these unsatisfied owners might opt to rent out their farms. Second, land may be rented by owners who have reached the end of their active work life.

A.1. The Land Rental Market – LARMA

The new LARMA component was embedded into the UCA sub-model. A description of LARMA can be found in Bert et al. (2010). Briefly, LARMA is a hybrid model that relies in part on neoclassical economics. Nevertheless, LARMA addresses some of the drawbacks of the neoclassical approach by being integrated into an ABM that involves heterogeneous agents interacting in a dynamic environment. LRP formation in LARMA assumes economic equilibrium. The simulated LRP is that which maximizes the amount of hectares transacted in a cropping cycle.

LARMA's formation of LRP involves three consecutive steps: (a) identification of potential farmland supply and demand; (b) formation of both a "Willing to Accept Price" (WTAP) and a "Willing to Pay Price" (WTPP); and (c) calculation of a Market Clearing Price (MCP) that becomes the LRP for the cropping cycle being simulated. LRP depends, on one hand, on the WTAP of owners renting out their land due to (i) lack of capital (ii) dissatisfaction with recent economic progress, or (iii) end of active work life. Potential landlords base their WTAP on the estimated profits they could achieve by operating their own farms instead of renting them out. LRP also depends on the WTPP and the working capital of potential tenants (i.e., farmers with surplus capital). Potential tenants base their WTPP on their desired gross margin for the upcoming cycle. Although LARMA does not include bilateral trading between agents, it involves other interactions (e.g., farmers monitor the economic outcomes achieved by their peers) that lead to adjustments in the agents' willingness to pay or accept certain land rental prices.

A.2. Mechanisms leading to farms being rented out

In an earlier PM version, farms were rented out only by owners who did not have sufficient WC to crop their land. In the current version, even farmers with sufficient WC may rent out their farms if (i) they are unsatisfied with their recent economic progress and (ii) the market offers an attractive rental price.

During the determination of potential land supply, owners assess whether they are satisfied with their economic progress in the recent past. This is intended to produce an extended timeframe for the assessment of achieved outcomes. Assessment of satisfaction is very similar to the "*N* out of *M*" mechanism that triggers the search for alternative land uses in the "Land Allocation" model process (Bert et al., 2011). First, a farmer computes his economic progress rate (PR) over the *M* most recent cropping cycles – PR is defined as the relative increase in WC between two consecutive cycles. Second, the farmer compares this PR to a target Minimum Progress Rate (MPR) that is the minimum of two alternative values: (i) an MPR defined for each farmer at initialization (e.g., 5%) or (ii) the average PR of the farmer's spatial neighbors. This second option was defined to avoid considering as unsatisfactory cycles with low economic returns that arise from unfavorable contexts (e.g., poor climate conditions) affecting all farmers similarly. If a farmer's PR is higher than his MPR in *N* out of *M* cycles (e.g., in 3 of 5 years, consecutive or not), the farmer is satisfied; otherwise, they is unsatisfied and will consider renting out his farm. Thus they need to form a WTAP. Dissatisfaction with progress does not automatically imply that a farmer will rent out their land. They will do so only if LRP is higher than their WTAP. For this reason, the final supply of rental farmland can be determined only after the formation of LRP based on preliminary supply estimates.

A second process by which farms are added to the rental land supply was included in the latest PM version. Some owners reaching retirement age may rent out their farms. Details are discussed in Section 3, as the need for this process emerged from the calibration and validation stage. After the supply and demand of rental land are determined, the remainder of the UCA sub-model is identical to that described in Bert et al. (2011).

Appendix B.

Gross Margin (GM) series used in the simulations are shown in Table B1 for: (a) soybean, (b) maize and (c) wheat. GM series were compiled from three different sources: two trade magazines (Agromercado and Márgenes Agropecuarios) and official Ministerio de Agricultura, Ganadería y Pesca (MAGyP) statistics. Values are expressed in constant US dollars per hectare (in April 2009).

Table B1
Series of gross margins (GM) used in the simulations. GM series were compiled from three different sources: two trade magazines – Agromercado (Agmdo) and Márgenes Agropecuarios (MA) – and the official Ministerio de Agricultura, Ganadería y Pesca (MAGyP) statistics. Values are expressed in constant US dollars per hectare (in April 2009). Crop yields assumed for GM calculations differ between sources: Agmdo assumes realistic yields for each cropping cycle. MA assumes average yields for groups of cropping cycles for which production technologies remain constant. Yields used by MAGyP for the calculation of GM were not available.

Cropping cycle	Soybean			Maize			Wheat		
	Agmdo	MA	MGAyP	Agmdo	MA	MGAyP	Agmdo	MA	MGAyP
1988/89	271.0	367.0	149.8	233.0	269.0	226.4	155.0	144.3	158.4
1989/90	125.0	187.0	177.3	100.0	164.3	143.8	67.0	103.4	167.0
1990/91	192.0	205.9	322.5	108.0	188.1	247.4	−15.0	162.5	−13.4
1991/92	282.0	334.3	357.0	248.0	317.9	256.9	133.0	130.3	189.8
1992/93	370.0	343.0	293.0	256.0	298.1	201.2	213.0	167.0	242.8
1993/94	390.0	428.3	350.3	249.0	437.7	345.5	163.0	232.8	185.5
1994/95	397.0	424.7	267.5	335.0	374.0	270.1	303.0	205.3	196.4
1995/96	415.0	305.5	530.9	363.0	500.4	791.1	508.0	313.4	428.6
1996/97	589.0	617.8	384.1	755.0	885.4	360.5	213.0	521.5	138.3
1997/98	722.0	684.4	433.4	386.0	478.5	326.4	217.0	391.8	179.2
1998/99	498.0	352.3	259.6	251.0	278.8	328.9	169.0	182.7	81.3
1999/00	260.0	250.2	263.4	265.0	297.5	237.3	58.0	225.8	70.6
2000/01	410.0	387.1	264.4	167.0	224.3	176.5	119.0	202.2	186.1
2001/02	362.8	362.8	298.5	285.0	386.1	311.5	120.0	177.8	149.9
2002/03	358.2	358.2	456.3	234.0	492.3	332.8	206.0	274.8	138.0
2003/04	397.1	397.1	434.5	155.0	407.9	357.2	211.0	269.3	290.4
2004/05	607.0	441.8	359.0	309.0	411.3	120.3	48.0	207.2	56.2
2005/06	308.0	353.2	297.4	93.0	252.4	158.0	99.0	120.5	73.0
2006/07	382.0	361.9	409.0	251.0	343.5	545.2	170.0	171.5	126.3
2007/08	437.0	447.5		392.0	506.1		262.0	310.5	
Median values for period:									
90/91–99/00	393.5	347.7	336.4	260.5	346.0	298.3	191.0	215.6	182.4
00/01–07/08	389.6	375.0	359.0	242.5	397.0	311.5	145.0	204.7	138.0

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