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An interdisciplinary framework for the development and analysis of crop models

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Abstract: Development and use of crop models has become an interdisciplinary field with the increase on one hand of the biophysical knowledge and the development of numerous dedicated software platforms on the other hand. This trend calls for formalizing the integration of the disciplinary contributions of scientists having different expertises needed in crop modelling : agronomists, mathematicians, software scientists.
We propose an interdisciplinary framework to : (1) describe the model with different expert domain knowledge, (2) identify bridges to help scientists of different domains to work together on the same model, (3) give a methodological basis (engine) for crop model studies. This theoretical framework is thus based on the integration of: (1) the agronomic domain describing the simplified functioning of soil-plant systems and the associated hypotheses; (2) the mathematical domain giving the system of equations and its properties and (3) the software domain defining the software components and their relationships.
We show how these views can be specifically defined for the description and studies on crop models, how they are related to each other, and how this framework integrates some relevant concepts on integrated modelling. We finally illustrate the use of the framework for building a new crop model (a pea crop model) by changing an existing one (a wheat crop model).

Keywords: modelling framework, interdisciplinary framework, crop model, agronomic model, mathematical model, software model.

1 INTRODUCTION

The expression crop models hides an interdisciplinary perspective behind the use of the word model. It is often reduced to the software tool used to simulate the crop biomass production depending on different parameters and input variables: soil, climate, management practices, etc. However when an agronomist analyzes the results of a crop model, he/she starts to question whether the choice of crop processes selected for their specific application corresponds with their expert knowledge. An applied mathematician on the other hand questions how the systems of equations is solved, how the system parameters have been estimated, how the results are sensitive to uncertainty. A computer scientist concentrates on the software design and architecture, and looks for bugs. Each of these different specialists questions the model from their own perspective. Beyond this example of model evaluation, we want to stress that all three disciplines-agronomy, mathematics and software engineering science- have a major role to play when dealing with crop models development.

Today dedicated software platforms (i.e. integrated modelling platforms) make the development of a crop model potentially quicker and easier than in the past, especially when they integrate graphical interfaces and graphical programming functionalities. Some of the most sophisticated tools, such as Simile (Muetzelfeldt and Massheder [2003]) propose a visual modelling environment to specify graphically the model and to reduce the effort required to implement it. This is undoubtedly a progress and a gain in time that enables the modeler to keep more energy for the other aspects of crop modelling process such as the statement of hypotheses and the mathematical model formalization. These aspects remain irreducible when dealing with crop modelling, since the increase of knowledge does not reduce the difficulties and limitations of biological prediction at macroscopic spatial and temporal scales (crop scale and daily time step) with limited calibration and validation data. These issues were already pointed out in Monteith [1996] and Sinclair and Seligman [1996]: it is impossible to identify all possible factors influencing crop performances. This agronomic model validity is therefore tightly linked to the hypotheses stated on local relevant crop processes and on the data available to parameterize and evaluate the model. We add another sense of mathematical validity associated with a crop model. The translation of the selected processes into a mathematical dynamical system is not unique, and the properties of the system once built can play a major role to interpret the simulation results : typically a very unstable system of equations can propagate uncertainties of the input data in such a way that any prediction based on experimentally calibrated parameters can not be reasonably accurate. Finally the software validity relates to code quality and to software testing. The latter ensure that the simulation software runs properly with software components consistently translating the concepts and equations of the agronomic and mathematical models.
These different aspects of model validity are often interlaced for a model developed in a platform. Hence it is more difficult to identify the origin of the wrong results of crop models as they can originate from each of the three domains. This fact stresses the need of a triple domain -agronomy, mathematics and software engineering- disciplinary framework. More generally, we designed an interdisciplinary framework with the purpose to: (1) describe the model with different expert domain knowledge, (2) identify bridges to help scientists of different domains to work together on the same model, (3) give a methodological basis (engine) for crop model studies.

2 AN INTERDISCIPLINARY FRAMEWORK BASED ON A TRIPLE DOMAIN VIEW

We introduce our framework based on views from three disciplinary domains and their respective activities. We also describe the associated links between these views.

2.1 Description of the triple domain view framework (Figure 1)

Agronomic Modelling. We start the description by considering the agronomic view of the crop model. We refer to it as the "agronomic conceptual model" as introduced by Wery et al. [2009], Rapidel et al. [2006] and Lamanda et al. [2010] by analogy with the conceptual models related to Information Systems. Its main properties are described in the following.
The main outcome of this agronomic modelling process is to formalize a scientific question into a conceptual model with an abstraction level not directly linked to mathematical or software representations. The principles governing its construction are those of the system analysis theory (Rabbinge and De Wit [1989]) and the different steps proposed in Wery et al. [2009] to design it are:

- Formulation of objectives
- Definitions of the limits of the system
- Conceptualization of the system
- Quantification of input relations

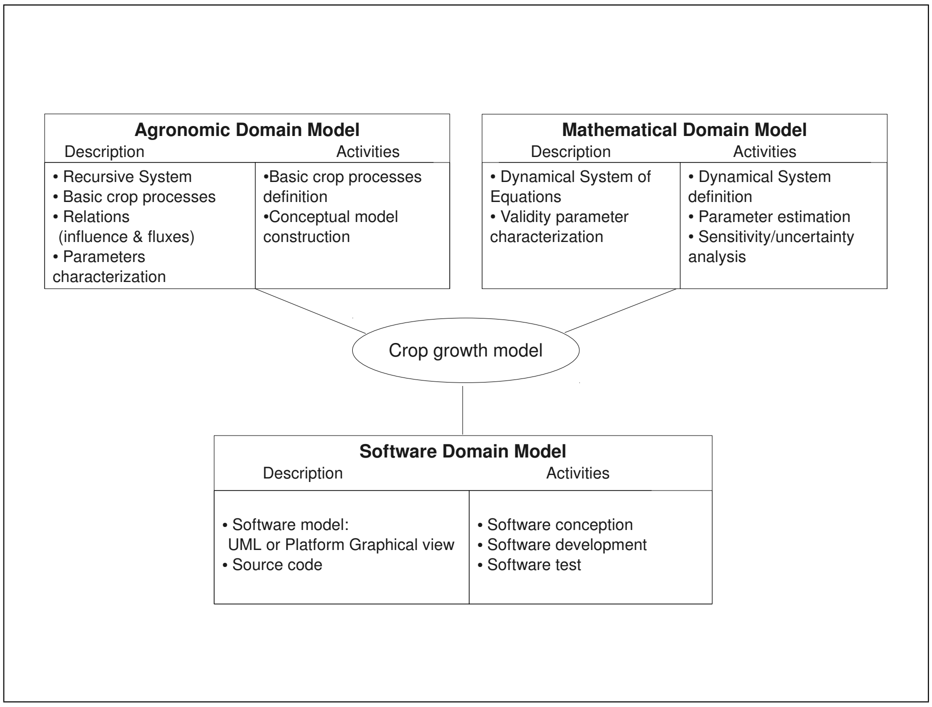

Figure 1: The three dimensions of a crop growth model and the associated formalizations and development activities

This agronomic conceptual model expresses the scientific question to be solved by modelling. It is the initial explicitation and specification step of the model development in the framework. As a disciplinary tool, it can also be used independently of the numerical model development: for instance it can help agronomists to develop an in-field comprehensive analysis of yield components (Rapidel et al. [2006]).It might also be the correct initial level of abstraction for a collaborative model design when agronomists and other scientists such as hydrologists, biologists or economists gather knowledge from their expertise field.
This property explains why its representation is more general than the diagrams used is some visual programming approaches. For instance, it contains to the definition of the main basic crop processes (Adam et al. [2010b]) needed for the model application. But it also states explicitely the hypotheses and includes a detailed description of the validity domain of subsystem model and parameters. It clarifies whether the model parameters have to be measured only once or for each new soil-climate-genotype combination. An example of a diagram extracted from a conceptual crop model based on crop processes is given in section 3.
Inside the framework, it plays the double role of product of the initial crop system analysis to be used by agronomists and communication tool between scientists involved in the whole modelling process.

Mathematical Modelling. The mathematical part of the triple disciplinary framework comprises the description in the mathematical form of the dynamical system and some associated activities such as dynamical system definition and analysis.
The role of mathematical expertise in the modelling process applied to the crop modelling shall indeed not be underestimated, even if the classical structure of crop models, which are classically composed by a set of explicit difference equations, leads to straightforward resolution of the system by direct time integration. This structure is also characterized by a very large number of parameters coming from the detailed accumultaive description of crop processes (for example more than one hundred in the STICS Model (Ruget et al. [2002]). In that sense, despite the simple structure of the dynamical system of equations, the mathematical object resulting from numerous biophysical processes can be complex. The need to work on this complexity with expert knowledge makes necessary the mathematical representation of a crop model inside our framework.

A disciplinary activity related to the mathematical field is the study of model structure to reduce the number of its parameters or more generally to improve its mathematical properties. Another example is the statistical analysis that focuses on the response of the system to variations of its input. This is commonly addressed by sensitivity and uncertainties analysis of a model, and which may require expert skills when the system is large and its resolution time consuming (Wallach et al. [2006]).

Software Engineering and Modelling. The third view including a disciplinary model representation and some associated activities deals with the software engineering domain.
Here we do not want to enumerate the different possible ways to implement a crop simulator with or without a software platform. The software model of this view (see Figure 1) denotes different objects depending on the simulator implementation: (1) in the most sophisticated integrated tools, it is the graphical model representing the model components as in Simile (Muetzelfeldt and Massheder [2003]), STELLA (Richmond [2001]); (2) in a standalone application coded using an object oriented language it can be the UML class diagram of the software application, and (3) in its most crude form the model is reduced to the source code.
Even if we have chosen not to point out one method rather than another, the need of interdisciplinary communication required by our framework promotes tools having explicit software models underlying the source code. This objective is closely related to the paradigm of Model Driven Architecture, applied to crop modelling in Papajorgji and Pardalos [2006]. Its goal is to separate the platform independent conceptual models of the software components written in an UML-based approach, from the executable code that can be at least partly automatically generated by an engine using the UML model. It is also the same objective of the so called Declarative Modelling approaches implemented in Simile and STELLA : the model structure is stored in an open text file and is thus separated from the rest of the source code needed to run simulations. The benefits of such approaches are recognized in the software engineering field for the gain of reliability, productivity and modularity (Papajorgji and Pardalos [2006]). Moreover it fits with our framework objectives of interdisciplinary exchanges, as we will see in the coming section.

2.2 Links between framework domain views (see Figure 2)

The three disciplinary representations of the crop model have to be connected in order to make the framework operational, as suggested by the double sided arrows in figure 2. The detailed formulation of the dynamics of crop processes is made in the mathematical domain view, as well as the formalization of the relations (influence, regulation) that are mentioned in the agronomic conceptual model. The connection between the mathematical model and the software model is made by the numerical methods needed to solve the equations of the mathematical system. Finally the software model is created from the agronomic and the mathematical models, and should be as much as possible a consistent transcription of the agronomic conceptual model into a software architecture.
Like the agronomic conceptual model, abstraction in the software architecture helps the communication between experts from the three disciplines and the sharing of their own model definition: this is necessary to strengthen the global model and to sort out problems specific to each domain when a simulation gives wrong results. Such software models (sometimes called software conceptual models) however shall not be identified with the two others model representations even if there are links as we already mentioned. It is indeed very unlikely that the agronomic expert knowledge can be embedded in the software view of a model. The validity hypotheses attached to the agronomic conceptual model are not building block of the software construction. The same remark holds with the fine mathematical properties of a crop mathematical model : they are unlikely to be better expressed than in the mathematical language.
Going one step further towards the formalization of the relations among the disciplinary domain views leads to the concept of component approach. Classical component approaches are related to software elements, which typically wrap a crop process in a software unit. The latter can be switched in the same software modelling solution and in theory exchanged between different scientists (Donatelli et al. [2009], Wang et al. [2002], Jones et al. [2001], Bergez et al. [2009]. This approach is necessary to help code re-use but often entails a common software platform or simu-

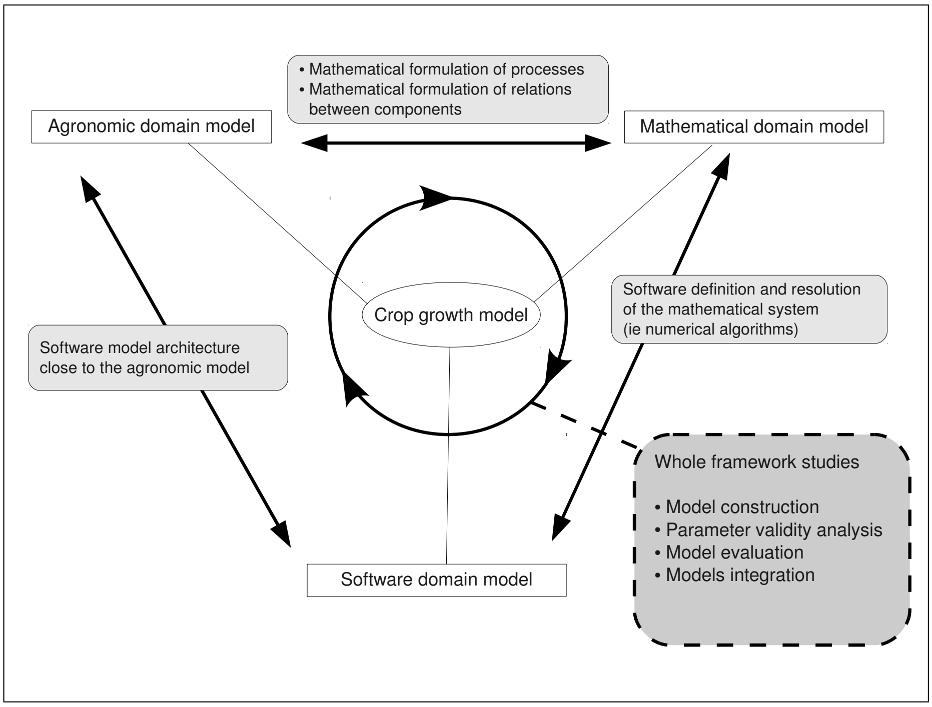

Figure 2: Triple domain framework: links between domain views and activities. The double sided arrows represent the relations between the three different model formalization. The cycling circle depicts the iterative aspect of model development across the three views. The dashed box enumerates some activities that can be propagated through the three domain views.

lation engine in order to be able to integrate the software elements, as in Simile (Muetzelfeldt and Massheder [2003]), APES (Donatelli et al. [2009]), APSIM (Wang et al. [2002]) or VLE (Quesnel et al. [2009]). This is a limitation to knowledge sharing inside the international crop modelling community. However using our approach, a component can be defined and shared at different disciplinary levels: at the conceptual level between agronomists working on different platforms, at the mathematical level between mathematicians working on the same processes, or at the software level for scientists working on the same platform.

3 AN EXAMPLE OF THE FRAMEWORK APPLICATION

The framework can be used for a wide class of problems on crop models that require interdisciplinary expertise. In the dashed box in Figure 2, we mentioned the general examples of model construction, model evaluation and model integration.
In this section we detail the application of the proposed framework on the following question : how can we build a new crop model from an existing one? More precisely, this example takes a wheat simulation model and aims at deducing a pea growth simulation model (Adam et al. [2010b]).
The framework gives a straightforward procedure based on the successive use of the three domain views to get an implementation of a pea growth simulator from an existing wheat model. This is a one loop process because at this level we do not consider the data validation of the new simulator, which would require an iterative procedure between the different models as suggested in the central loop in Figure 2. The framework based procedure that we have successfully used (Adam et al. [2010b]) can thus be summarized as follows :

- at the agronomic level: analyse the conceptual model with expert knowledge to identify which basic crop processes and relations must be added or removed and modified through for instance the change of the species specific parameters

- at the mathematical level: define or update the mathematical definition of the processes and the new relations
- at the software level: propagate these changes into the software components through the software platform (CROSPAL (Adam et al. [2010a]) in this example)

This process is illustrated in figure 3, with the comparison between the diagrams of two conceptual crop models and the required changes coming from the previous analysis. The agronomic analysis of the basic crop processes to be modelled leads to the addition of the new component Nitrogen Fixation. This change implies adding a new module in the software model. On the other hand, the change in the Leaf Development process only requires to change the mathematical formulation in an existing software module.

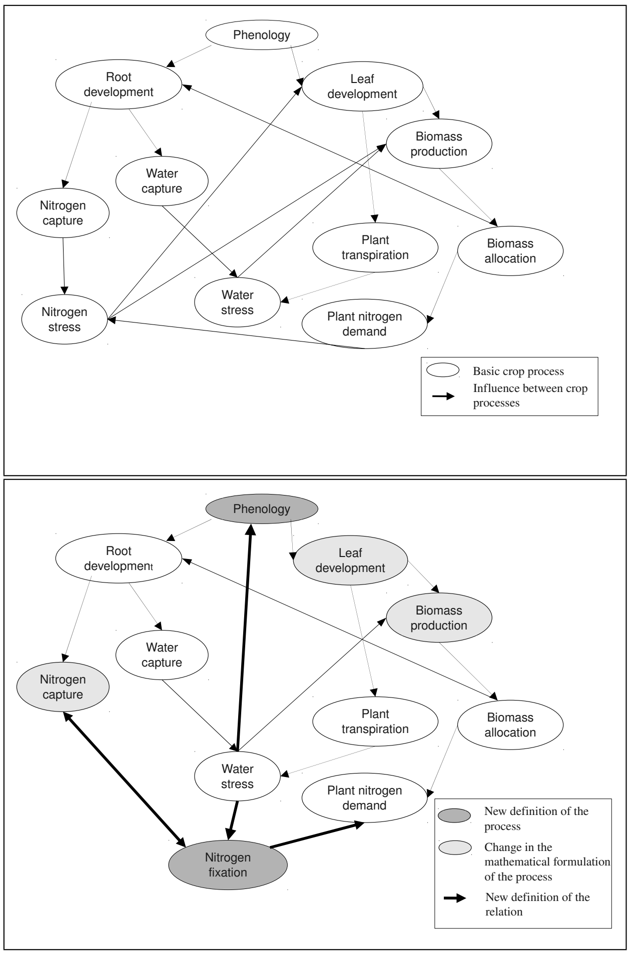

Figure 3: Illustration of the changes needed to develop a pea crop simulator from a wheat crop simulator. Using the framework, the changes are firstly analysed on the conceptual model. The associated modification are shown on the right side with different colours depending on the models to be mostly affected : light grey for the mathematical model, dark grey for both the mathematical and software models.

4 Conclusion and discussion

We have introduced a framework for the interdisciplinary development and analysis of crop models. We have shown how to define the three main domain views and what are the related disciplinary activities. We have explained the relations between the different roles and shown how

the representations are connected. How to go one step further and formalize semantically these relations is still an open question in our framework. To this aim, evaluating the possibilities to establish formal links between the disciplinary representations through ontologies as in Villa et al. [2009] seems promising.
This framework does not rely on an unique integrated software tool for several reasons. Promoting a software tool would unbalance the equilibrium toward the software aspects, and be incompatible with the necessary freedom for experts to use the most adapted tool required by their activity. For instance, applied mathematicians will be keen to use popular scientific software like Matlab or R. Moreover, such integrated tools would necessarily limit the framework to a concrete definition. Conversely an original benefit of our framework is its ability, as a theoretical tool, to suggest methodologies to tackle new problems on a crop model.
The complete assessment of the operational value of our framework is an ambitious task that will probably reveal some limitations. Nevertheless, as we learned from the presented example (pea crop model) and from other case studies currently under progress, the triple disciplinary framework already appears to be a stimulating tool for crop models formalization between agronomists and a facilitation tool to initiate collaborations between agronomists, applied mathematicians and computer scientists. This is why we believe that separating the three domains representations can ease international collaboration on disciplinary questions (for instance exchanges between agronomists on concepts and processes that can be made on conceptual models) while allowing an improved interdisciplinary collaboration around crop models based on the same software platform or environment such as Simile (Muetzelfeldt and Massheder [2003]) APSIM (Keating et al. [2003]), SEAMLESS (Van Ittersum et al. [2008]), RECORD (Bergez et al. [2009]).

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