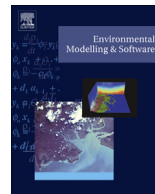




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journal homepage: www.elsevier.com/locate/envsoftAgricultural production systems modelling and software: Current status and future prospects[☆]Dean P. Holzworth^{a, *}, Val Snow^b, Sander Janssen^c, Ioannis N. Athanasiadis^d, Marcello Donatelli^e, Gerrit Hoogenboom^f, Jeffrey W. White^g, Peter Thorburn^a^a CSIRO Agriculture Flagship, Australia^b AgResearch, New Zealand^c Alterra, Wageningen UR, Wageningen, The Netherlands^d Democritus University of Thrace, Xanthi, Greece^e Consiglio per la Ricerca in Agricoltura, Bologna, Italy^f Washington State University, United States^g USDA-ARS, United States

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ABSTRACT

During the past decade, the application of agricultural production systems modelling has rapidly expanded while there has been less emphasis on model improvement. Cropping systems modelling has become agricultural modelling, incorporating new capabilities enabling analyses in the domains of greenhouse gas emissions, soil carbon changes, ecosystem services, environmental performance, food security, pests and disease losses, livestock and pasture production, and climate change mitigation and adaptation. New science has been added to the models to support this broadening application domain, and new consortia of modellers have been formed that span the multiple disciplines.

There has not, however, been a significant and sustained focus on software platforms to increase efficiency in agricultural production systems research in the interaction between the software industry and the agricultural modelling community. This paper describes the changing agricultural modelling landscape since 2002, largely from a software perspective, and makes a case for a focussed effort on the software implementations of the major models.

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1. Introduction

It has been just over a decade since Donatelli et al. (2002) summarized the 2nd International Symposium on “Modelling Cropping Systems” in the special issues of European Journal of Agronomy. They presented a synopsis of the status of cropping systems modelling at that time, with some indicators of possible future developments. At that time, crop modelling was dominated by DSSAT (Jones et al., 2003), APSIM (Keating et al., 2003), CropSyst (Stöckle et al., 2003), EPIC (Izaurralde et al., 2006) and STICS (Brisson et al., 2003).

Over the past decade, cropping systems models have expanded in scope to become agricultural production systems models that are used in a range of applications:

- a) climate change and adaptation (Elliott et al., 2014; Fraisse et al., 2006; Kalaugher et al., 2013; Moore et al., 2014; Pearson et al., 2008, 2011; White et al., 2011),
- b) food security (Carberry et al., 2013),
- c) policy assessment (Bezlepkin et al., 2010; Bryan et al., 2011; Ittersum, 2009),
- d) aiding the development of tools for farmers and/or policy applications (Cichota et al., 2012; Hunt et al., 2013; Komarek et al., 2012; Parsons et al., 2011; Shafuallah, 2012),
- e) farmer advice (Adam et al., 2010; Carberry et al., 2002; Hochman et al., 2009; Oliver et al., 2012),
- f) resource use and efficiency (Liu, 2009; Qureshi et al., 2013; Ranatunga et al., 2010; Salazar et al., 2012),
- g) plant breeding (Hammer et al., 2010; Hoogenboom et al., 2004; Messina et al., 2011),
- h) bioenergy (Persson et al., 2010a, 2010b),
- i) livestock and mixed crop-livestock systems (Berntsen et al., 2003; Lilley and Moore, 2009; Rotz et al., 2005) and

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- j) yield gap analysis (Hochman et al., 2012; Liu et al., 2012; van Ittersum et al., 2013; van Ittersum et al., 2003).

The breadth of applications demonstrates that agricultural production system models are serving a societal need of evidence provision and that they have grown to maturity from research prototypes of the mid-1990s to application workhorses in the early 2000's. The last decade has also seen major investments from research agencies and governments around the world, for example, the commitment of three organisations in Australia to develop APSIM, the European Commission's Joint Research Centre's (JRC) commitment to develop yield forecasting applications with WOFOST, and the International Food Policy Research Institute's (IFPRI) use of DSSAT with the IMPACT model for policy analysis. In the same period, many applications of models became embedded within specific research or policy organisations, where they were routinely used in policy or business decision making. For example, applications for yield forecasting were part of the JRC's activity on Monitoring Agricultural Resources (www.mars.info) and as part of USAID's monitoring of Famine Early Warning Systems Network (www.fews.net). Also, extensive publications on impact evaluations with crop models were included as part of the IPCC's chapters on impacts of climate change of agriculture (www.ipcc.ch). A commonality among these examples is that they use or interpret the model outputs at larger regional scales, using either grid or administrative-region based approaches. Some crop models were incorporated in farm management advisory programs (www.yieldprophet.com.au; www.agroclimate.org).

Although these applications demonstrate that agricultural production systems models are able to serve particular needs, there remains a large untapped potential for further application and development, especially in domains that are currently underserved, including food security, policy assessment, farmer advice, and human health and nutrition. Robust applications in these new domains require that models are further developed. Much remains to be done on improving the quality and/or scope of the underlying science of plant responses to elevated CO₂ and temperature extremes and the flow-on effects of these to soil carbon and nutrient dynamics. A more detailed representation of spatial heterogeneity and its impacts on crop and environmental performance is also of crucial importance. In these domains, it is important that the crop models link to models of other disciplines (such as pests and diseases, economics, hydrology and supply chain management) and include a broad representation of all sorts of crops present on the farm. The models must be broadened to include the livestock components that are critical parts of many production systems and food security globally and at the smallholding level, as well as speciality and underutilized crops, such as vegetables and tree fruits.

The objective of this paper is to outline our positioning for the next phase of agricultural systems modelling, defined as the production elements (and constraints) of a farming enterprise (e.g. cropping, livestock, pastures). We will evaluate developments over the last ten years, both from a modelling and Information and Communications Technology (ICT) perspective; and by proposing a research agenda and approach for the decade to come. In our view, there is an opportunity to rethink past strategies, as ICT is opening up massive opportunities for further development that will benefit model users through more robust models or models that are more efficient or more agile to develop and apply. These opportunities include improved computational performance (e.g. via cloud computing techniques or parallel processing methods), and rapid community-driven application development with a focus on mobile devices, equipped with sensors and positioning possibilities.

In Section 2, we present examples of what the agricultural modelling community has accomplished in the past decade. We have seen advances in broadening the application domain, the modelling scale and the formation of new research coalitions for addressing international and global challenges. At the same time, we identify some long-standing software problems and failures that we detail in Section 3. Research has been hampered by legacy code and the lack of good software engineering principles. We still struggle to obtain robust datasets to be used for benchmarking. In Section 4, we present new and emerging areas of research. Based on the papers submitted in this Thematic Issue and other relevant literature, we explore recent innovations in agricultural models and frameworks. Then, in Section 5, we attempt an overview of new challenges and opportunities for research. The paper concludes with a vision outlining the activities needed to shape the short to medium term future.

2. Strengths and achievements

The application domain for agricultural models has evolved significantly in the past decade. As the title of this paper suggests, the emphasis is now on agricultural systems rather than cropping systems. A decade ago the focus was on improving on-farm crop productivity. This is still important today but the modelling community has become increasingly interested in greenhouse gas (GHG) emissions, levels of soil carbon storage, food security, risks of pest and disease losses, livestock production, and climate change mitigation and adaptation. While models addressing these issues existed a decade ago, integration across domains is new. This expanding application domain has led to additions to existing models; new algorithms, processes and capabilities have been added, where each of the models include more crops, more environmental outputs. Outside of the existing models, several new models have been developed to address different aspects of these themes; Rivington and Koo (2010) found that there were about 250 models available. Most prominent were the developments of APES (Donatelli et al., 2010), AQUACROP (Hsiao et al., 2009; Raes et al., 2009; Steduto et al., 2009), INFOCROP (Aggarwal et al., 2006). New modelling frameworks have also been created; OMS (David et al., 2013), RECORD (Bergez et al., 2014), BioMA (<https://en.wikipedia.org/wiki/BioMA>) as an extension of APES; and OpenMI (Gregersen et al., 2005; Knapen et al., 2013).

The expanding application domain has also necessitated a change in modelling scale. Large area scenarios of agricultural productivity at the farm, country, continental and global scale are now commonplace and have required a spatial, parallel simulation capability to be added to the models and frameworks or the construction of model wrappers that provide this capability. Interestingly, all of the models and frameworks are still point based (1D models) although some models now allow multiple points to be run simultaneously with dynamic interactions (APSIM, CropSyst). This capability is important for grazing system applications (Snow et al., 2014), whole farm management (Moore et al., 2014; Rodriguez et al., in press), and water movement and storage within properties (Brennan et al., 2008) or across landscapes (Paydar and Gallant, 2008). The scale of applications has also moved to the small scale, with crop improvement programs seeking to incorporate genetic models for traits into biologically dynamic crop models to predict gene–phenotype relationships (Cooper et al., 2009; Hammer et al., 2010; Messina et al., 2011; White et al., 2008a).

The last decade has also seen the development of a large consortium of agricultural, climate and economic modellers, working together to improve adaptive capacity for major agricultural regions around the world. The Agricultural Model Intercomparison

and Improvement Project AgMIP (Rosenzweig et al., 2013) uses model inter-comparison and improvement, future climate scenarios, economic scenarios and an ensemble of models to develop and explore adaptation strategies. It has brought together modellers from different organisations, countries and disciplines into a coherent entity to work toward a common set of goals. In some ways, this project is a successor to the International Consortium for Agricultural Systems Applications (ICASA) (Jones et al., 2001) but has a different membership and focus, concentrating on climate change related applications. In addition to AgMIP, there are or have been other large groups of agricultural modellers that formed during the past decade; SEAMLESS (van Ittersum et al., 2008), the APSIM Initiative (www.apsim.info), MACSUR (www.macsur.eu), and the DSSAT Foundation (www.dssat.net). All have fostered, to varying degrees, a cross collaboration of ideas, tools and methodologies, and sharing of code by moving towards open source.

These collaborations evidence increasing willingness by agricultural modellers to work together and to span disciplines. We have observed in the past decade that agricultural modellers have become more receptive and open; both as individual teams and together as a community. Individual teams have realised the limitations of working in isolation and the need for cross-fertilising ideas. At a community level, it seems that the broadening scope of the studies revealed the need for cross-comparison of methods and tools.

3. Weaknesses and long-standing problems

One of the strengths of the scientific literature is its role in the peer review of scientific methods and analyses. This leads to sound scientific ideas being routinely reused and adopted among the community. This doesn't happen as much for software model implementations; the *Environmental Modelling and Software Journal* fills this niche to some extent but many software developers don't routinely submit papers that describe software implementations or processes. So rather than presenting a summary of weaknesses as evidenced by the scientific literature, we focus, instead, on software issues, a subject not normally covered.

While the application domain has broadened, and modeller networks have expanded, the software implementations of the major models (e.g. DSSAT, EPIC and APSIM) have largely remained as they were a decade ago. FORTRAN is still used as the programming language for the biophysical models in DSSAT, EPIC, and much of the current release of APSIM (note that STICS and CropSyst have been re-implemented in C++ and APSIM is currently moving to.NET). FORTRAN remains dominant primarily due to its legacy as the predominant language used by scientists and modellers from its inception in the 1950s through to the 80s and 90s when much of the science or biological part of today's simulation models were initially developed. The models themselves are typically large constructions each containing their own implementations of very common approaches to modelling crop and soil processes.

Most models still rely heavily on their legacy code. This reliance comes from significant past efforts spent to build those model components, which to date are still performing and functioning well, and are heavily used by many scientists as critical parts of ongoing research delivery. This legacy code however, is typically written using procedural languages, which limits the options for evolving the code toward a more modern code base. In addition, most young programmers are not familiar with this style of programming, as software engineering curricula has long moved on to new paradigms that are easier to manage. At the same time, most of the legacy code is at best poorly documented, and access to source code is often restricted to a limited group of developers. When combined with a lack of investment and resources over a long

period of time, the code base becomes almost impenetrable for new scientists who want to extend the functionality or create new models. As a consequence, the burden of model maintenance and evolution falls to a small pool of scientists, often long involved in the development of the software.

The principle of software reuse, something the software industry has long recognized as highly desirable, has not been largely realised in the field of agricultural systems modelling. The legacy of large model constructions hinders reuse and swapping of processes. Most models are locked in data and model structures that were designed decades ago. When the models were initially developed, programming languages were less flexible and computer hardware constraints (e.g. disk space, RAM) significantly affected software implementation decisions. The reuse of processes was not a design goal or consideration and community development of models was not even contemplated. Most processes were also coded with an emphasis on the underlying science and not necessarily software efficiency. New features, extensions, and tools were typically wrapped around those monolithic cores, making the software maintenance more complex with every release. At the same time, there was minimal standardisation of model inputs or internal structures. Although the emphasis of the ICASA Consortium was standardization of model inputs and outputs, this was not well received in the modelling community (Hunt et al., 2001; White et al., 2013). Each team made its own structural assumptions and this resulted in the exchange of data among models becoming a programming burden. Most models reached a high level of maturity with large user communities and significant investment of effort into input and experimental evaluation datasets. The combination of these issues makes changes in data and model structures extremely costly for both the developer and the user.

Code reuse is usually only seen at the relatively large scale of a whole crop or soil. For example, some of the frameworks have wrapped models to enable their reuse in multiple frameworks. The IRRI rice model ORYZA (Bouman and van Laar, 2006) is one such example. A version of ORYZA runs in both DSSAT and APSIM via a wrapper layer that abstracts the idiosyncrasies of each framework behind an application programming interface. Another example is the Root Zone Water Quality Model (RZWQM) that now includes the crop components of the DSSAT crop models (Ma et al., 2006, 2005). The wrapping approach to model reuse has some advantages in that the wrapped model is a known entity (although it still requires testing as it will interact with differing parts of the new framework) and can often shortcut intellectual property issues. However, this type of reuse has been limited because of the difficulties in wrapping very large model constructions where the soil and crop calculations are entwined. For widespread code reuse, a much finer level of granularity is required.

There is one framework where this level of reuse is directly supported; BioMA is a software framework that directly supports reuse and composition of small modules (<https://en.wikipedia.org/wiki/BioMA>). To date though, none of the major modelling groups have looked seriously at it as a way of reusing modules, although water-limited versions of CropSyst and WOFOST were re-implemented (Donatelli et al., 2014; Stella et al., 2014). At the same time, a cross comparison of four integrated modelling frameworks (ESMF, CCA, OMS and OpenMI) using example models from the hydrology domain (Lloyd et al., 2011) concluded that integrated modelling frameworks are invasive, as they introduce new dependencies to software implementations, and in contrast lightweight frameworks are needed. To this end, Athanasiadis and Villa (2013) considered Domain-Specific Programming Languages as an enabler for reuse in integrated environmental modelling.

The agricultural modelling community also fails to give software testing sufficiently high priority. The software industry has long

viewed testing as critical to the performance and robustness of released software. Agile software techniques like test-driven development and unit testing are used widely by the industry to reduce the number of defects that need to be fixed post release. The lack of adoption in the agricultural modelling community is likely due to scientists doing the model coding, who have not been trained in formal software testing techniques. These scientists typically have tight milestones to deliver outputs and outcomes, so testing is given a much lower priority. There are some exceptions: Holzworth et al. (2011) outline the testing regime employed in APSIM, while BioMA utilises pre- and post-condition testing throughout the framework.

Another recurring point of failure in models is that maintenance of documentation and software/code has not been considered a core research outcome, so adequate resources are rarely allocated (by either institutions or funding bodies) to such activities. Investment in good documentation and software/code maintenance would enhance model use, and is an important aspect of maximising the value of the investment in models. It has been estimated to roughly cost US \$15–20M to design, implement, evaluate and deploy SWAT and RZWQM (David et al., 2013). The original development cost of DSSAT, under the auspices of International Benchmark Sites Network for Agrotechnology Transfer Project (IBSNAT), was US \$10M over a period of 10 years. Likewise, the APSIM Initiative estimates that it costs approximately US \$1M per year to maintain and extend APSIM. Most research grants are application or issue-driven within which model development and implementation is typically a side product. Communities working with the current suite of models have difficulty in sourcing resources for software development and improvements in a sustainable manner. This results in software that is maintained in an *ad-hoc* fashion to the point where often the best way forward in improving the software base is to start from scratch. However, such a decision results in the loss of investment in processed/formatted input data, ancillary tools to support the usage of specific models and the wealth of user experience and expertise in the original model. As an example AgResearch, a pastoral research organisation in New Zealand, experienced such a situation when they decided to move from the traditional modelling base to APSIM. The decision to change was primarily driven by the desire for greater collaboration in model development and application than was possible using a proprietary modelling platform. There was also a need to reduce the research expenditure on model infrastructure and maintenance. The transition was more expensive and time consuming than initially anticipated. This was partially because APSIM had not been used in pastoral systems to any significant extent, and the new usage required a combination of changes in the underlying science as well as the framework infrastructure. Also needed for the transition was the translation of soil and weather databases as well as user tools to aid applications such as sensitivity analysis. Of course the users also needed time to fully understand the representation of the processes and the assumptions implicit in the models in APSIM. These development needs were met through additional investment from AgResearch and through support from the existing APSIM community. Five years after the initial transition into APSIM, AgResearch's decision has paid off and resulted in much greater collaboration, both within New Zealand and internationally. The adoption of the more flexible and collaborative modelling framework has both increased research outputs per unit of investment in modelling and fostered greater demand for modelling to be integrated into field-based experimental projects. Perhaps the AgResearch case shows a way forward: only with strong collaborations can we sustain and maintain software infrastructures.

In summary, the history of the development of agricultural production systems models has been generally characterised by

gradual, often *ad hoc* improvement and extension of the models, with groups adding 'new' modules that have been previously implemented elsewhere. This has led to an expansion in the number of crop and soil processes considered within the models but with little attention being paid to other important processes, such as modelling pest-diseases, perennials, and bridging the gap between simulated and actual on-farm yields.

4. Recent innovations and upcoming challenges

4.1. Reflections from this Thematic Issue

The Special Issue of European Journal of Agronomy in 2003 contained a mixture of model description papers, papers describing innovative applications of models, as well as a synthesis anticipating likely future needs. The highlighted needs included a broadening of the need to consider environmental and ecological aspects of farming and for modelling frameworks that facilitate development and flexible application. More than a decade later, we see that these issues are still very active. Below we try to identify trends from the papers submitted to this Thematic Issue, but also from recent literature.

Five of the papers in this Thematic Issue (Bergez et al., 2014; Holzworth et al., 2014; Kang et al., 2014; Raes et al., 2014; Stöckle et al., 2014) contain updates to model description papers originally published in 2003. Importantly, this Thematic Issue also contains descriptions of new models of plants in agricultural systems (Brown et al., 2014; Huth et al., 2014; Ma et al., 2014) and new modelling platforms for grape vines (Martin-Clouaire et al., 2014), livestock systems (Herrmann et al., 2014), pests and diseases (Bregaglio et al., 2014; Whish et al., 2014) as well as new modelling systems for simulating the small-holding farm systems common in developing countries (Franke et al., 2014; Le et al., 2014). Almost all the submissions mentioned climate change, food security and/or ecosystem services although this might be expected given the nature of the call for submissions. Ewert et al. (2014) review models for their suitability for assessment studies of climate change impact and risk.

Approximately half the submissions include some aspect of interoperability of, or between, models or modelling frameworks. This theme arose in many guises ranging from models that are frameworks themselves (Holzworth et al., 2014; Stöckle et al., 2014), that are applications within frameworks (Bergez et al., 2014; Brown et al., 2014; Donatelli et al., 2014; Herrmann et al., 2014; Martin-Clouaire et al., 2014; Whish et al., 2014) or that plead the need for frameworks with greater interoperability for various reasons (Elliott et al., 2014; McNider et al., 2014; Porter et al., 2014; Snow et al., 2014). The issue of interoperability was originally flagged by Donatelli et al. (2002). With recent efforts in this area, it might seem that the original symposium spurred interest and development in this area – an area that has enabled a much greater range of applications.

Another theme that emerged from the submissions to the Thematic Issue was the need for a multiple or parallel simulation capability, which arose from a range of different purposes. These ranged from spatial issues, from small areas of heterogeneity caused by the behaviour of grazing animals (Snow et al., 2014), to the need for multi-paddock simulations to capture farm performance when that performance is dependent on the interaction of several paddocks rather than just the aggregation of many single paddocks (Herrmann et al., 2014; Holzworth et al., 2014; Moore et al., 2014), to several papers (Balbi et al., 2014; Elliott et al., 2014; Kang et al., 2014; Le et al., 2014; Machwitz et al., 2014; McNider et al., 2014; Porter et al., 2014; Raes et al., 2014; Stöckle et al., 2014; Yu et al., 2014; Ziadat et al., 2014) concerned with

some aspect of many-site or gridded applications of simulation models. This rise in demand for gridded applications does not seem to have been anticipated in the 2003 Special Issue.

While ensemble modelling has been in common usage by climate modellers for some time, as a simulation method it is relatively new to agricultural production system modelling. However, it is quickly emerging as a useful way for modellers to interact with each other to address emerging issues, such as on climate change through the AgMIP Project (Asseng et al., 2013; Rosenzweig et al., 2013). Ensemble modelling features in this Thematic Issue in the forms of process ensembles within models (Donatelli et al., 2014) and small ensembles of crop models (Marin et al., 2014), as well as the recognition in many other papers of the need to maintain model usability for deployment in ensemble modelling. The Thematic Issue also includes discussion of provisions for ensemble modelling. Agricultural ensemble modelling is currently bringing together large teams of people, and there is a need for an ontology that describes the data available for model 'proving'. Kersebaum et al. (2014) build on the ontology put forward by Rosenzweig et al. (2013).

One issue that (Donatelli et al., 2002) did discuss was the likely increase in complexity of the simulation models. In this Thematic Issue, this increase in complexity is very evident and has arisen from a range of different sources. Huth et al. (2014) and Raes et al. (2014) discuss the need to develop or parameterise crops with little or minimal information while (Wallach and Thorburn, 2014) show an alternative approach to evaluate model performance. Archontoulis et al. (2014) and Brown et al. (2014) consider the need to rapidly estimate values for phenological parameters in crop models. There is also increased complexity as the need to simulate perennial crops (Herrmann et al., 2014; Holzworth et al., 2014; Ma et al., 2014), including tree and vine (Bergez et al., 2014; Martin-Clouaire et al., 2014; Moriondo et al., 2014) species, results in carry-over effects across production years. APSIM, CropSyst, DSSAT and EPIC are all able to simulate such carry-over effects. The issue of carry-over effects is also important for the models focussed on grazed pastoral systems (Herrmann et al., 2014; Snow et al., 2014), but these models face the added complexity of the need to model, in some form, the animal as an additional trophic level. Whish et al. (2014) also discuss the issues associated with additional trophic levels but here they are concerned with the pests and diseases of cropping systems. In modelling more complex systems, there is also increased demand for improved methods to model or consider management decisions as described by Martin-Clouaire et al. (2014) and Moore et al. (2014). It seems likely that this emergence of more complex modelling problems has partially arisen from increased capability of the simulation models and their user interfaces, but it is also likely that as we address emerging issues associated with ecosystem services (Balbi et al., 2014; Le et al., 2014) in the face of climate change.

Despite its importance, assessment of model performance and/or uncertainty received little attention in the Thematic Issue. Ensemble modelling provides insights into uncertainty (Asseng et al., 2013; Rosenzweig et al., 2013) as demonstrated by one paper in the Thematic Issue (Marin et al., 2014). However, there was only one paper (Wallach and Thorburn, 2014) dealing with statistical approaches to quantifying performance in agricultural production systems models, and none on statistical approaches to quantifying uncertainty. Uncertainty and sensitivity analyses are computationally intensive so the slow run-time and large number of parameters in many agricultural systems models makes uncertainty and sensitivity analyses challenging. However, these analyses are becoming common in some other applications of agro-ecosystem models (e.g. greenhouse gas emissions; Wang and Chen, 2012) and we would expect to see these analyses

increasing in applications of agricultural production systems models. Approaches to make the analyses more efficient in agricultural models are likely to be beneficial.

A notable omission to the Thematic Issue was papers describing advances in gene-to-phenotype modelling. Breeding companies have increasingly recognised that dynamic crop models may have a role to play in improving the efficiency of their crop improvement programs. Theoretical studies have suggested that incorporating empirical genetic models for traits into dynamic crop models is possible (Cooper et al., 2009; Messina et al., 2011). For this to work though, the phenotype of a trait needs to be linked its underpinning genetic control (Chenu et al., 2009; Hammer et al., 2006; White and Hoogenboom, 2003). While this adds a level of complexity to the parameterisation of the resulting model, the breeding companies see a quicker route to identifying promising breeding strategies. This approach has been demonstrated with dry bean, soybean and wheat in DSSAT (White et al., 2008a) and sorghum in APSIM (Hammer et al., 2010).

4.2. Data harmonisation innovations

All agricultural modelling groups require access to field trial data for development, evaluation and comparison purposes. Each modelling group stores and manages that data in different ways and in different formats. The DSSAT group use the ICASA data standard which began development in the 1990s (Hunt et al., 2001; White et al., 2013). The other groups use a combination of text and XML files, spreadsheets and databases. These different approaches hinder direct usage of that data by different modelling groups and that creates an entry barrier to new collaborations.

One of the goals of AgMIP is to directly compare different modelling approaches. To facilitate this, the ICASA data standard was adopted as the storage format, and AgMIP members developed translators and tools to convert the format to and from the various crop models (Porter et al., 2014). This standard carefully describes agronomic and crop management data, but its data dictionary approach appears to be sufficiently extensible to other related domains such as livestock, pasture and pest/disease systems. This will be tested soon within the AgMIP community. This standard allows an ensemble of models to use the same data format, facilitating direct comparison. Multi-model ensembles allow modellers to investigate model algorithms, comparing and contrasting approaches, ultimately leading to model improvements. Ensemble modelling is impossible without the sharing of experimental and global data as common pool resources. Data compatibility can only be achieved by adopting a common vocabulary and format, and then either extending models to read that format or translating the data into a model readable format. AgMIP chose the latter approach for most of the models it uses. The exception is CropSyst; it was modified to read the AgMIP standard format as an additional option. While this has greatly facilitated direct model comparison, challenges still exist. Models of different complexity within the ensemble have different data requirements and representations of processes. The AgMIP experience has mainly focussed on crop models to date, and there will be challenges when broadening the applications to include models of other systems, e.g. grassland and livestock systems. Even within the relatively limited domain of crop models, format differences have meant that some translators have needed to convert detailed experimental data into simpler inputs for the model. Models do not always share the same terminology, and several times the meaning of a single term has proven to vary across models. Semantic disambiguation and universal definitions remains as the main challenge that the AgMIP community undertakes for the creation of a common vocabulary for exchanging data.

AgMIP is not the only consortium to attempt the data harmonisation challenge. SEAMLESS invested significant resources into data accessibility by models and individuals. When multidisciplinary teams are formed, a shared understanding of concepts and the meaning of data can be difficult to achieve. SEAMLESS took the approach of developing a shared set of ontologies to semantically link models (Athanasiadis et al., 2009; Janssen et al., 2011; Villa et al., 2009). The ontology contains metadata describing the data it contains and specifies data communication across the models in SEAMLESS. However, the SEAMLESS scope was constrained to the project specifics, and as such the community was confined within the consortium. It was not even attempted to include in the process communities outside Europe, or to develop a culture for achieving results on a volunteer basis. As noted above, the AgMIP and MACSUR programs are investing in developing ontologies (Kersebaum et al., 2014) with the aim that they are quite general to, at this stage, crop modelling.

4.3. Software development advances

The demand for spatial use of models has led to the development of techniques and tools that wrap individual models. This can be at the small spatial scale, for example precision agriculture and variable rate applications (Basso et al., 2011; Nijbroek et al., 2003; Thorp and Bronson, 2013; Thorp et al., 2008), or it can be large scale at a high resolution (Elliott et al., 2014; Zhao et al., 2013). While the models remain point-based, the frameworks run multiple points in parallel. As the models themselves remain intrinsically point-based, in that they respond to a particular combination of soil and weather, they are being wrapped and executed in parallel to simulate broader scales. The larger scale (country, continental and global) execution environments typically contain some aspects of large data storage and processing, parallel and cloud based computing. The computing infrastructure required to run point models in massive gridded applications is reasonably straight forward; computer clusters and parallel computing are now commonplace. A key challenge is in how the individual point models are parameterised in these gridded applications, and whether these points interact with each other. Climate, soil and management information are required at each grid cell, but accurate, detailed data are almost never available. Climate data are now becoming more readily available as gridded data (current and future climate scenarios) (Weedon et al., 2011), and soil profiles can be synthesised effectively at each grid cell (White et al., 2008b; Wu et al., 2010a, 2010b). However, defining management interventions for each cell is a major constraint, especially for pastoral systems where multi-paddock interactions should be considered within each grid point. Interpreting the results from complex models can also be difficult and some researchers (Baveye and Laba, in press; Donatelli et al., 2011) consider that a better approach might be to use models that have a broader level of abstraction and suggest that the complexity of some models can hinder analysis. This model fit-for-purpose question is usually overlooked in favour of adopting an off-the-shelf model, likely one with which the researchers have some experience, regardless of its possible complexity misfit. This is a common pitfall in integrated modelling (Laniak et al., 2013). Some decisions are often a trade-off between the 'right' model for the task and the easiest model for the researchers to use acknowledging that CPU time is significantly cheaper than researcher time. As a modelling community, we do not yet have a good framework to decide which models are more suitable to use for any given application or assessment.

The need for integration of crop models with livestock and pests/diseases has led to the need for more flexible ways to precisely control the interaction of many land units in the same

simulation (Moore et al., 2014). This emerging requirement for interconnectedness has implications for framework design. The APSIM and BioMA frameworks support such applications by allowing the user to specify multiple points (locations) within a simulation and then describe the flows of data between these points or management interventions on specific points via a scripting language. This approach is flexible for small-to medium-sized applications but does not scale easily to a large number of points, and the management logic to control interventions can become very complex (Moore et al., 2014).

Despite the broadening of the agricultural application domain and the new science and data standards that support this broadening, the software implementations of the leading models remain largely unchanged. Some have been (partially) redeveloped using object-oriented languages (APSIM, STICS, CropSyst). Some now use component-oriented techniques (BioMA, APSIM to some extent). Also, the use of software process tools like continuous integration, version control, unit testing are becoming more commonplace (Holzworth et al., 2011). There also hasn't been a sustained effort by the agricultural modelling community to make the frameworks more accessible. An exception to this is APSIM, which is open-source for non-commercial use with its source code available on the web. DSSAT is also currently experimenting with sharing the source code of the model through GitHub. A decade ago, van Ittersum and Donatelli (2003) noted that most simulation models were relatively inaccessible and reflected the developer's specific way of defining objects. This situation has changed little over the subsequent decade. Many of the models remain incompatible with each other with little or no reuse of models or code between frameworks. For example, a model from APSIM cannot run in DSSAT, CropSyst, STICS, or other frameworks without wrapping or recoding. Instead, the same algorithms are recoded many times, for each framework. One protocol that was developed in the last decade is OpenMI (Gregersen et al., 2007) aiming to connect old FORTRAN style hydrological models quickly and easily, but its adoption in the agricultural modelling space has been limited. There are several reasons for this. The first is that independently of its generic scope, OpenMI was inspired by hydrological modelling. OpenMI, now an Open Geospatial Consortium candidate, seems more suitable for models with geographical reference, and seems to contain too much unnecessary overhead for point- and time-based simulation models with fixed structure, as most agricultural models are. For a more detailed discussion of the modelling framework overheads, see (Lloyd et al., 2011).

4.4. Model reuse: why is it so hard?

Model reuse has improved little over the last decade. Many crop models are based on similar radiation use efficiency (RUE) approaches, yet they have been implemented in different source code bases or in fundamentally different ways. Likewise, many of the soil models use either a "tipping bucket" or a Richards' equation approach but all have different implementations of these (Donatelli et al., 2014). Different implementations of the same algorithm can lead to subtle differences that aren't immediately apparent. For example, DSSAT and APSIM both have a tipping bucket water balance model and some of their parameters look similar but have subtly different meanings. What drives model reuse that is not being captured by the agricultural modelling community?

Many crop models remain black boxes with little documentation of how they work. Also, most of the models are large constructions of soil, crop, and nutrient components. It is well known in the software industry that smaller units of computation are easier to understand and reuse between different projects. Small units of computation can be aggregated into larger constructions to

form models as we generally known them in the agricultural community. There are some notable movements towards finer levels of model granularity in the agricultural modelling community (e.g. APSIM, STICS, CropSyst, and DSSAT) but in all cases, the potentially reusable units are programmed in different ways that are incompatible with one another. Even when using modern software techniques, this is a consequence of placing the focus on frameworks rather than on reuse. The requirements to foster model re-use at low granularity are specific and basically ignored (Donatelli et al., 2014) even though there is no ongoing cost associated with low granularity. Closed source model frameworks also hinder reuse and further exacerbate the black box effect through not being able to examine (and possibly improve) the inner workings of a model or algorithm; a model architecture exposing semantically rich interfaces with examples of unit tests and usage would greatly be a significant step forward.

Institutional and intellectual property boundaries have also impeded collaborative model development and reuse, although this is changing. The APSIM Initiative was created in 2007 with a goal of encouraging shared development of agricultural models, providing open access to source code and validation data sets (Holzworth et al., 2011). This Initiative has made significant inroads into encouraging organisations in Australia and New Zealand to focus on a shared vision for agricultural model development. Likewise, the BioMA framework has seen collaboration between modelling teams in Europe and the United States and the SEAMLESS and MACSUR projects have done similarly within Europe. More recently, the AgMIP consortium has attempted to bring together all these groups into a modelling collective. Perhaps strong endorsement by AgMIP for open software may finally provide the environment where model and process sharing and reuse is realised.

5. Potential roads ahead

To pursue a broadening agricultural domain, there needs to be a radical improvement of the models, making them more 'applicable' to a wider range of questions, much better at representing agricultural systems, having much more objective and reproducible calibration and validation, and, from an ICT point of view, being more scalable and easier to apply in new directions. If agricultural production systems models do not take this next step, the discipline is likely to only remain attractive as a scientific domain for developing some small extensions and building scientific careers, as in a societal sense we have covered more-or-less what is required to address the historical questions for which the models were developed: the current applications are all that is needed for those questions.

Currently, several paths are being explored simultaneously to increase efficiency in agricultural production systems research at the intersection between the software industry and agricultural modelling. The first is the development of one or more component based libraries of frequently used algorithms (modelling approaches implemented at fine granularity), that can easily be combined and have standard ways of connecting to data across applications. An example of this can be found in BioMA platform (<https://en.wikipedia.org/wiki/BioMA>), and this could ultimately lead to the current situation in agent based modelling, which has Netlogo (<https://ccl.northwestern.edu/netlogo/>), Swarm (<http://savannah.nongnu.org/projects/swarm>) and Repast (<http://repast.sourceforge.net/>) as established modelling tools, with common constructs for developing an agent based model. The strength of this approach is that it allows community collaboration around a common 'trusted' base, allowing applications to be built on shared components. The lack of similar tools in the agricultural space

implies that agricultural modellers may need to develop an agreement on model structure and conceptualization. Some modellers, though, may not like a single design, particularly if source code is not open source and is poorly documented and tested.

A second approach is the development of higher level programming languages which enable the fast programming of new models, programmed as mathematical equations, instead of using traditional programming languages. This revisits the notion of declarative modelling approaches (Muetzelfeldt and Massheder, 2003), but moves forward from the graphical representation of equations with stocks and flows, to a development environment where modellers would code just the equations, and leave the implementation issues to the modelling framework. The general requirements for domain-specific programming languages for environmental modelling have been introduced by Athanasiadis and Villa (2013). One of these is cross-compilation for different environmental modelling frameworks. As an example, consider a model of finer granularity written once in a domain-specific language, which can subsequently be compiled and incorporated into a variety of models. One approach for achieving this is via the OASIS XML Interchange Language (www.iseesystems.com/community/support/XMILE.aspx). Members of the OASIS standards technical committee are working to develop an open XML protocol for sharing interoperable systems dynamics models and simulations.

Similar lessons are learnt from other disciplines. In economics for example, there is rarely a discussion on model re-use. Most economic models are implemented in languages like GAMS (www.gams.com) and SAS (www.sas.com), where every researcher just re-implements their model depending on the context and scientific questions at hand. These models can be shared with others, as most of the source closely resembles the mathematical equations, however there is very little reuse. These languages offer an easier entry point for novice model builders but do not help with the framework issues of model connectivity and sharing. An exception to this is the generic implementation of a bio-economic farm model (Janssen et al., 2010).

A third approach is to use the current suite of models as they are, in an ensemble of models (Asseng et al., 2013; Elliott et al., 2013) using standardized data exchange formats (Porter et al., 2014; White et al., 2013). The models can then be offered as services in a web-enabled architecture, with large computing facilities, to enable a diverse range of large scale applications (Elliott et al., 2014). This solution is employed (partly) in the genomics domain (for example the iPlantCollaborative, www.iplantcollaborative.org), whereby combining modelling approaches and data services lead to rapid advances in the analyses of the genome. The strength of this approach is that it takes full advantage of past investments in the implementation of models and extensions. A clear weakness though is that the large building blocks hinder transparency and so remain black-boxes, obscuring close comparisons with other models and evaluation of model performance. Even model users operating at the large scale should concern themselves with model fit for purpose, something that is difficult to do with large model constructions (Stella et al., 2014).

Aspects of each of these approaches are currently being explored as is demonstrated by the manuscripts submitted to this thematic issue. Arguably, given the three approaches outlined above, it is impossible to select one as being more desirable. Instead they should be considered complementary with each providing a part of the future road map. What is required though is that a sufficiently large community of modellers, research funders, application-driven researchers and software engineers come together and continues to work on providing robust models, tools and infrastructure for the future.

During the past decade we have also observed several advances in model integration and cross-disciplinary science, which is slowly changing the practice of modelling itself and the requirements that are put on the modeller in terms of interaction and demonstrable impact of the work. Firstly, integrated modelling (Laniak et al., 2013) is becoming a common practice where models are linked over domains and are often considered for assessment of food security, climate change and ecosystem services. Second, more modelling is done in a participatory setting (Voinov and Bousquet, 2010) where modellers, together with stakeholders, evaluate scenario options and develop a common understanding of the problem and the system being modelled. Third, with the advance of big data, sensor data, and open linked data, there exists more possibilities for model evaluation studies (Bennett et al., 2013; Matthews et al., 2011), where the over or under complexity of the model for the question at hand can be studied (Refsgaard et al., 2007; Warmink et al., 2010).

6. Necessary conditions to facilitate the road ahead

Agricultural production systems models will continue to be applied to new application areas for supporting research and farm advice on a broad range of farming systems, from small-holder farmers to large industrialised agricultural holdings. To fully realise their potential, much greater emphasis on the software aspects of the models and frameworks is needed. Evolving many of the current models to these new disciplines and applications will be impossible without a significant investment in better software.

Rather than rewrite existing models or build a single, unified, model framework (something that past experience has shown is not practical), a renewed focus on the software design and development processes should be fostered within the modelling community to better enable cross comparison of approaches and sharing of algorithms among existing frameworks. Activities that need further efforts include;

- a) Examination and extension of existing approaches to writing framework and platform independent algorithms are needed. An approach for writing algorithms that can easily be incorporated into existing frameworks would go a long way towards reuse. Fine granularity is an important design consideration when model improvement is the goal. For maximum reuse, algorithms should be small (e.g. radiation interception, root growth, runoff, soil water evaporation) rather than a large composite (e.g. a whole crop or soil).
- b) Further exploration of meta-languages (e.g. XMILE) seems warranted to avoid coding these algorithms for a specific language or framework. Algorithms coded using a meta-language could then be implemented into traditional programming languages via language translation.
- c) Guidelines for documenting algorithms are needed that describe the data requirements, the science of the algorithm and expected outputs. There also needs to be improvement in training material for the existing models to better equip novices in model usage.
- d) An emphasis on the testing of algorithms and models is needed to improve their robustness and behaviour under different conditions.
- e) There needs to be continued development of a publicly available set of benchmark data sets (and a standard for their description) that can be used for evaluation of the models and algorithms at different scales. This will greatly help with examining model improvements.
- f) An appropriate mechanism needs to be developed to provide credit when publicly available data and algorithms are used.

For this ideal to be realised, the community needs to be better organised as a practice-oriented learning network with a willingness to share ideas, approaches and algorithms. Teams need to be multidisciplinary with agricultural modellers and experimentalists working alongside of software engineers so as not to be limited to existing technology but to be able to take advantage of ICT technologies to formulate models that fulfil emerging requirements, not past ones. This requires teaching curricula of agricultural sciences and post graduate courses to be more cross disciplinary, particularly with respect to ICT skills and competences (e.g. methods such as agile and user-centred design). This will help modellers and IT specialists to work together more effectively.

7. Discussion and conclusion

The advantages of a renewed focus on the software engineering dimensions of agricultural modelling are clear. The efforts listed in the previous section would a) allow more cross comparison at a finer level of granularity; b) provide better transparency of alternative approaches and c) lead to more openness amongst agricultural modellers, leading to better sharing ethics (open access and open source). Open, transparent and free software processes, models and tools has been shown to promote more open collaborations among the agricultural modelling community.

Examples of this are already beginning to happen but a global focus has not eventuated because of drivers both internal and external to the modelling community. There is resistance from some groups where their primary goal is to further science through PhD and post-doctoral research or they are dependent on meeting contractual milestones. This requires a degree of confidence that the modelling framework will be sufficiently robust so as not to endanger research. The funding environment in which agricultural modellers work also hinders core software development and maintenance activities. Grants are approved based on promised outputs and outcomes not by the transparency and reusability of core model units. Further, tight project milestones have led to the belief that specific model implementations could be extended to cover different needs, taking away the urgency of improving simulation tools. However, it is increasingly clear that the old monolithic simulation technologies can be fragile, hard to maintain, let alone extend, and (through lack of documentation and non-transparent design) can be unacceptably reliant on a single person (or a small team) for continued operation. These conditions can present an unacceptable level of risk to a research organisation and so can be used as an impetus for change – indeed this was the primary reason for AgResearch moving from its existing framework to APSIM. An updated modelling technology can reduce the effort and improve the robustness of the transfer of new science to an operational model. In doing so, it can considerably reduce the time required to meet societal demands for acceptable or adoptable solutions via the development of new tools. We would argue that while ten years ago it was a vision of only a few, it is rapidly becoming a more pressing need.

Although efficient software frameworks proposed by Donatelli et al. (2002) could be part of the success story, a community effort is needed that is based on trust and openness for sharing of code and data among the various modelling groups. The initial activities of AgMIP, MACSUR and the APSIM Initiative have provided mechanisms and potential incentives for these types of activities. However, these efforts are only the beginning and need to be nurtured and broadened. Key to the future success of agricultural modelling will also be the ability to recruit young scientists that are interested in this field and are willing to move these approaches to the next level as part of their professional careers and who are rewarded by their respective employers, either in the

public or private sector. The field of ICT is moving rapidly and our stakeholders, ranging from farmers to policy and decision makers, are now demanding that research must catch up with their needs and provide the information via push technology to their smart hand-held device. In a future world, our models need to evolve to meet these changing demands.

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