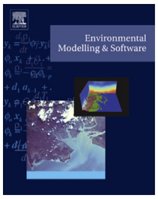
Environmental Modelling & Software xxx (2014) 1–9

Contents lists available at ScienceDirect

Environmental Modelling & Software

journal homepage: www.elsevier.com/locate/envsoft



A generic framework for evaluating hybrid models by reuse and composition – A case study on soil temperature simulation[☆]

M. Donatelli[a,*], S. Bregaglio[b], R. Confalonieri[b], R. De Mascellis[c], M. Acutis[b]

[a] Consiglio per la Ricerca e la sperimentazione in Agricoltura, Centro di ricerca per le colture industriali (CRA-CIN), Via di Corticella 133, I-40128 Bologna, Italy
[b] Università degli Studi di Milano, Department of Agricultural and Environmental Sciences – Production, Landscape, and Agroenergy, Cassandra Lab, Via Celoria 2, I-20133 Milan, Italy
[c] Institute for Mediterranean Agricultural and Forestry Systems (ISAFOM), National Research Council (CNR), Via Patacca 85, I-80056 Ercolano, NA, Italy

ARTICLE INFO

Article history:
Received 9 January 2014
Received in revised form
14 April 2014
Accepted 16 April 2014
Available online xxx

Keywords:
Model composition
Model comparison
Model development
Composite indicators

ABSTRACT

We evaluate modelling solutions built composing different modelling approaches. Modelling of soil temperature was the case study, evaluating modelling solutions against a multi-year, multi-location database of field recorded data. Widely used simulation packages were re-implemented using advanced techniques, and nine new modelling solutions were built hybridizing across the original ones. Multi-metric indices were developed for modelling solution evaluation.

The hybrid solution implementing the Parton's approach (surface temperature) and the SWAT (temperature along the soil profile) led to the best compromise between agreement and robustness under the explored conditions. Differently, choices of soil water redistribution models caused a modest variability with respect to the simulation of soil temperature. The methodology presented allows providing clear indications about model choice and should be considered useful practice in model development.

The model libraries used to run the analysis are freely available for download, and they allow for further extension of the composition exercise.

1. Introduction

The term *model* is intended as an abstract representation of a part of the real word, and can be constituted by mathematical equations which are meant to capture the traits of system behaviour with respect to a specific objective of analysis. The term model is often overloaded in comparison to its specific structure: models range from very complex formalizations to a single equation, very often being compositions of many sub-models. Biophysical models in agriculture are no exception: what is commonly referred to as either crop or cropping system simulator is a set of interlinked mathematical representations of approaches which are abstractions of a single biological or physical process. They are called models, instead of the possibly more appropriate term *modelling solutions* (MSs), mostly because of the way they appear to the final user. Also, when they originated at the beginning of the 80s, their implementation was monolithic, often not making their discretization obvious in several sub-models. The need for a finer granularity of model units, to be reused at least to avoid duplication, has been a declared goal of the modelling community for many years (e.g., Argent, 2004). The seminal work of Leavesley et al. (1996) presents a pioneering work in the domain of agriculture. However, technological bottlenecks have made model reuse impractical for years, hence precluding what is at the basis of the concrete opportunity of model hybridization as a development practice. The crucial step forward to overcome technological constraints within a development environment has been given by modelling platforms (Argent and Rizzoli, 2004), but much work remains before such software infrastructures are adopted as mainstream modelling tools (David et al., 2013), even if the understanding of requirements is now noticeably articulated (e.g. David et al., 2013; Whelan et al., 2014). The separation of algorithms from data, the reusability of I/O procedures and integration services, and the isolation of MSs in discrete units have brought a solid advantage to development of simulation systems as shown by modelling frameworks such as APSIM (Keating et al., 2002; Holzworth et al., 2014) and TIME (Rahman et al., 2004). In such

---

[☆] Thematic Issue on the Agricultural Systems Modelling & Software.
[*] Corresponding author.
E-mail address: marcello.donatelli@entecra.it (M. Donatelli).

http://dx.doi.org/10.1016/j.envsoft.2014.04.011
1364-8152/© 2014 Published by Elsevier Ltd.

Please cite this article in press as: Donatelli, M., et al., A generic framework for evaluating hybrid models by reuse and composition – A case study on soil temperature simulation, Environmental Modelling & Software (2014), http://dx.doi.org/10.1016/j.envsoft.2014.04.011

systems, emphasis is placed on the development of the framework, and even new implementations of models have been strictly made targeting a specific one. Consequently, the reuse of modelling approaches has always required full re-implementation, very often even considering whole modelling solutions. However, there is no reason why a specific modelling solution should not test and possibly reuse several modelling approaches either being used in other model packages or newly developed, as part of its evolution. Some model packages already offer simulation options, for instance for models of evapotranspiration, or for soil water redistribution; but this as a result of the original design of a specific package, i.e. not importing and testing systematically, alternate modelling approaches. Shifting the focus from model frameworks to model units to build discrete, cross modelling platforms, software entities (e.g., Donatelli et al., 2006, 2009) has led to fine-granularity implementation of models, facilitating model hybridization.

If MSs are expected to be evaluated because one single process only may have changed, the methodology for the evaluation of such MSs should be verified. The methodology for model evaluation has evolved over time, considering different metrics (e.g., Bellocchi et al., 2002; Bregaglio et al., 2011). In all cases, however, evaluation has targeted MSs as immutable, except for versioning, discrete units. If we analyse the modelling core, as an example, of widely known MSs relevant to the plant–soil system, such as EPIC (Williams et al., 1989), APSIM (Keating et al., 2002), CropSyst (Stöckle et al., 2003; Stöckle et al., 2014), DSSAT (Jones et al., 2003), STICS (Brisson et al., 2003), we realize that they share many modelling approaches. However, even though "hybridization" across MSs occurred at least when a new one was initially built, importing and testing alternate options for the simulation of a single process never became a standard working methodology in model development. Evaluating whole MSs is perfectly adequate for the operational use of available discrete simulation packages, but it offers a confused picture if used to support model development, because it often does not provide clear indications of why a MS is performing better than others. This is not a minor issue, because even if building a MS is *per se* science, the research which can be more easily abstracted into modelling produces results mostly at process (i.e., sub-model) level.

In this study we want to explore model hybridization in terms of both the impact on predictive capabilities and of significance in model development, using well known model packages as starting MSs. We selected soil temperature as target state of the soil–crop system to be modelled.

Soil profile temperature (SPT) is of primary importance to simulate several processes: there is vast literature about the importance of SPT in driving the biochemical and physical processes involved with both the productivity and the sustainability of agricultural lands (e.g., Tsiros and Dimopoulos, 2007; Belviso et al., 2010). In spite of the importance of SPT data for the understanding of such a variety of processes, the availability of measured SPT data is mostly limited to research sites. In any case, as SPT is internal to the system of interest and driven by changes of several states, a measurement from a reference site cannot be used as an external driving force, like air temperature. The need for reliable SPT data led to the development of models for their estimation, characterized by different degree of adherence to the physical processes involved (e.g., Neitsch et al., 2011; Parton, 1984; Campbell, 1985). Among the inputs needed by such models, soil profile water content (SWC) plays a major role, given the peculiar thermal properties of water with respect to the ones of the other soil constituents (Campbell, 1985): an increase in the SWC causes an increment of the soil specific heat, because the specific heat of water ($4.18\ \mathrm{J\ g^{-1}\ K^{-1}}$) is higher than the one of quartz and clay minerals (0.75 and $0.76\ \mathrm{J\ g^{-1}\ K^{-1}}$); the thermal conductivity of water ($0.57\ \mathrm{W\ m^{-1}\ K^{-1}}$) is higher than the one of air ($0.025\ \mathrm{W\ m^{-1}\ K^{-1}}$), leading to an increase of the soil thermal conductivity at high SWC (De Vries, 1963). The lack of availability of consistent SWC measurements in large-area databases often requires SWC simulation with field parameterization as well (Basile et al., 2003). Hence, the simulation of SPT requires a MS to account for the processes involved, for which various modelling approaches are available, and this adds the complexity needed to avoid oversimplification in this proof of concept of the methodology.

The objective of this paper is to explore – primarily with a methodological perspective – a case of hybridization and evaluation of newly built and standard modelling packages for SPT simulation.

2. Materials and methods

2.1. Model composition: is some clarification needed?

When considering model composition, which is at the base of model development using different and alternate approaches, some terms have overloaded meanings, and at times confounded concepts can impact the activity. Firstly, two models are alternate options for simulating a process primarily if they estimate the same output. Other factors for now, that is, the number of parameters and even inputs required, are aspects relevant to the MS resulting from the use of a specific approach. One controversial aspect is the impact of estimating parameter values for MSs with a diverse number of parameters. When and if parameters can be estimated, as is often needed for instance for hydrological parameters in complex soil water models, another modelling layer is used. As far as such layer is available, its effectiveness impacts on the overall evaluation of the MS against reference data, and it should not be considered *per se* an absolute constraint in using the more complex approach.

Another controversial aspect in the composition procedure of simulation models relates to the time step of the modelling approaches being composed. We are not discussing here the time step of the MS, which should be adequate to capture the variability of the processes relevant to the scope of the analysis to be done. Rather, we discuss here the requisites which must be met in order to link two models, the first providing as output an input variable for the second.

The time constant (Leffelaar, 1999) is not the same for all processes simulated in MSs commonly used operationally, as the ones mentioned in the Introduction section. The time step of the MS determines when integration of state variables occurs for the whole system, and, in implementation terms, when different parts of the MS (either discretized as components or simply as routines of a structured programming implementation) communicate. Consequently, models at fine granularity can be composed if a given output matches the definition of the input required by another model. To illustrate the concept, if a model makes a variable available which is characterized by units, range of use, and description, and another model requires the same variable as input, the link should be considered correct (Donatelli et al., 2010). An evaluation should be made, prior to its use, regarding the correctness of the first model in producing the output, but once accepted that the model provides the specific output, use of that model should not be questioned in model composition. It should be evaluated, in an operational perspective and as discussed above, in the frame of the MS with respect to parameter and input availability. The above by no means states that all modelling approaches are equivalent, and several drivers may be considered by model builders in selecting a specific approach; however, it stresses that using a given (alternate) model is formally correct once accepted that the model produces the necessary output.

Model units were composed and run in this study using the framework BioMA (Donatelli et al., 2012), in particular leveraging on what are defined as Model and as Composition layers. Model components are implemented specifically for reuse (Donatelli and Rizzoli, 2008), making alternate approaches available for process simulation, thus facilitating the hybridization of MSs. Components are linked using the infrastructure provided by the Composition Layer, to transparently build and run MSs. The same action could have been performed with the other modelling platforms mentioned above, assuming all the modelling approaches mentioned were implemented at fine granularity to enable testing alternative solutions.

2.2. Modelling solutions

Nine MSs were built by combining (i) three different approaches for the simulation of SWC, (ii) two soil surface temperature (SST) models, and (iii) two models for the simulation of SPT (Fig. 1). Table 1 provides a description of the algorithms used in this study to simulate SST and SPT.

The simulation of crop growth and development was carried out using the model approaches of the generic crop simulator CropSyst (Stöckle et al., 2003), whereas evaporation was simulated with the approach proposed by Ritchie (1972) and implemented in the EPIC model (Williams et al., 1989). The EPIC approach for root water uptake was also used. CropSyst was chosen for its robustness (Confalonieri et al., 2010a), for its wide diffusion, and because parameterizations for

Please cite this article in press as: Donatelli, M., et al., A generic framework for evaluating hybrid models by reuse and composition – A case study on soil temperature simulation, Environmental Modelling & Software (2014), http://dx.doi.org/10.1016/j.envsoft.2014.04.011