# seamless

**System for Environmental and Agricultural Modelling;
Linking European Science and Society**

# Library of model components for process simulation relevant to production activities, Prototype 1 versions

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Partners involved: CIRAD, CRA, IAMM, IDSIA, INRA, PRI, UNIABDN, WU

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SEAMLESS integrated project aims at developing an integrated framework that allows ex-ante assessment of agricultural and environmental policies and technological innovations. The framework will have multi-scale capabilities ranging from field and farm to the EU25 and globe; it will be generic, modular and open and using state-of-the art software. The project is carried out by a consortium of 30 partners, led by Wageningen University (NL).

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# General part

## Objective within the project

**Provide a library of discrete software units implementing models / utilities for use both by third parties and to build the Agricultural Production and Externalities Simulator (APES)**

## General Information

Task(s) and Activity code(s):                  T3.2 – A3.2.9

Input from (Task and Activity codes):     T3.2 – A3.2.1/2/3/5/7

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Related milestones:                                M3.2.1

## Executive summary

In systems analysis, it is common to deal with the complexity of an entire system by considering it to consist of interrelated sub-systems. This leads naturally to consider models as consisting of sub-models. Such a (conceptual) model can be implemented as a computer model that consists of a number of connected component models. Component-oriented designs actually represent a natural choice for building scalable, robust, large-scale applications, and to maximize the ease of maintenance in a variety of domains, including agro-ecological modelling.

The modular approach was chosen to develop Agricultural Production and Externalities Simulator (APES). APES is a modular simulation system targeted at estimating the biophysical behaviour of agricultural production systems in response to the interaction of weather, soils and different options of agro-technical management. Although a specific, limited set of components is available in the first release, the system is being built to incorporate, at a later time, other modules which might be needed to simulate processes not included in the first version. The processes are simulated in APES with deterministic approaches which are mostly based on mechanistic representations of biophysical processes. The criteria for selecting modelling approaches are based on the need for: 1) accounting for specific processes to simulate soil-land use interactions, 2) input data to run simulations, which may be a constraint at EU scale, 3) simulation of agricultural production activities of interest (e.g. crops, grasses, orchards, agroforestry), and 4) simulation of agro-management implementation and its impact on the system.

This report presents the current state of development of the model components being developed for APES and for third parties use. The intended use and modelling capabilities of each component are summarized.

# Scientific and societal relevance

Creating a library of model components is a key part of developing a flexible simulation system that can be extended according to operational needs, and of sharing knowledge making available the relevant models for operational use. The modelling solutions and the implementation technology used are a realization of a goal being shared in the scientific community for more than a decade.

The envisioned impact is both on improving the use of resources by providing a way to avoid duplications, and by making available building blocks for quicker tool development, in order to match the demand from institutions and extension services.

# Specific part

## 1 Introduction

In systems analysis, it is common to deal with the complexity of an entire system by considering it to consist of interrelated sub-systems. This leads naturally to think of models as made of sub-models. Such a (conceptual) model can be implemented as a computer model composed of a number of connected component models. An implementation based on component models has at least two major advantages. First, new models can be constructed by connecting existing component models of known and guaranteed quality together with new component models. This has the potential to increase the speed of development. Secondly, the predictive capabilities of two different component models can be compared, as opposed to compare whole simulation systems as the only option. Further, common and frequently used functionalities, such as numerical integration services, visualisation and statistical ex-post analyses tools, can be implemented as generic tools and developed once for all and easily shared by model developers.

As a consequence of the above, in the last decade there has been an increasing demand for modularity and replaceability in biophysical model development (e.g. Jones et al., 2001; David et al., 2002; Donatelli et al., 2003, 2004), aiming both at improving the efficiency of use of resources and at fostering higher quality of modelling units via specialization of model builders in a specific domain. The modular approach developed in the software industry is based on the concept of encapsulating the solution of a modelling problem in a discrete, replaceable, and interchangeable software unit. Such discrete units are called components. A software component can be defined as "a unit of composition with contractually specified interfaces and explicit context dependencies only. A software component can be deployed independently and is subject by composition by third parties" (Szypersky et al., 2002). Component-oriented designs actually represent a natural choice for building scalable, robust, large-scale applications, and to maximize the ease of maintenance in a variety of domains, including agro-ecological modelling (Argent, 2004). The concept of developing modular systems for biophysical simulation has lead to the development of several modelling frameworks (e.g. Simile, ModCom, IMA, TIME, OpenMI, SME, OMS, as listed in Argent and Rizzoli, 2004, and Rizzoli et al., 2004), which allow making use of components by linking them either together or to a simulation engine. In fact, three major parts of the implementation of models are usually prototype specific, resource intensive, and prevent transferability: (1) data input/output procedures (e.g. input/output data handling, file management), (2) common services (e.g. state variables integrator, simulation events handler) and (3) graphical user interfaces (GUI). Modelling frameworks can play a key role to address these issues. First, the framework allows segregating the application-specific parts of simulations from the code employed to accomplish common tasks, thus greatly enhancing code reuse (Hillyer et al., 2003). Second, by defining the elements of the framework that actually contain the model implementation and how those elements are used, a designer can be presented with a clear path from conceptual model to simulation (Hillyer et al., 2003). Furthermore, avoiding the reimplementation of common services allows the concentration of resources on the development of simulation components.

Developing a simulation system adopting the component-oriented paradigm poses specific challenges, both in terms of 1) biophysical model linking, and 2) implementation architecture.

About the former, the component-based architecture demands for defining and implementing sub-systems which minimize the need for links to other components, minimizing also the need for repeated communication across components. Even when a system to be simulated is divided into sub-systems which minimize the need of communication across them, data exchange prior to integration within a time step is needed, hence requiring an articulated interfaced which allows for such calls. Another conceptual problem, often attributed to component-based systems as intrinsically and potentially prone to mix and match "everything", is shifted to components themselves using semantically rich interfaces which ensure that the linked variables are the correct ones. To illustrate the concept, if a component makes available a variable characterized by units, range of use, type and description, and another component requires the same variable as an input, the link can be considered correct if a check of the variable attributes can be successfully performed, whereas the correctness of using the variable as an input must be investigated within the component itself. The principle of applying "parsimony" is of course still valid in model building. For instance, there is no point in coupling two components in which the possible strong assumptions (and thus the limitations) of the former impose an unnecessary burden on the possibly extensive modelling capabilities of the latter; this, however, is a concept that applies both to monolithic and component based systems development. As always, it is the goal of both model application and system analysis which must suggest model choices, and this is independent of the type of implementation.

With regards to implementation architecture and use of modelling frameworks, there are two major problems: 1) the framework design and implementation must be optimized to balance carefully its flexibility and its usability to avoid incurring either a performance penalty or users having too steep a learning curve, and 2) developing components for a specific framework constrains their use to that framework.

In essence, two main options are available to overcome such problems. The most immediate is developing inherently reusable components (i.e. non framework specific), which can be used in a specific modelling framework by encapsulating them using dedicated classes called "wrappers"; such classes act as bridges between the framework and the component interface. The disadvantage of this solution is the creation of another "layer" in the implementation, which adds to the already implemented machinery in the framework. The appropriateness of this solution, both as ease of implementation and overall performance, must be evaluated case by case. The first prototypes of components developed in SEAMLESS for use in APES are based on this option, that is, developing non framework specific components which can be linked to different modelling frameworks, among which Modcom (Hillyer et al., 2003) is the one used in the current pre-release of APES. Other components under development, not available yet as discrete software units, are implemented as Modcom classes.

Regardless of the choice of developing framework specific or intrinsically reusable components, there is a basic choice which must be carefully evaluated prior to that and which is related, in general terms, to the framework as a flexible modelling environment to build complex models (model linking), but also to the framework as an efficient engine for simulation, calibration and simulation of model components (model execution).

Modern software technologies allow building flexible, coherent and elegant constructs, but that comes at a performance cost. Without even introducing Object Oriented Programming (OOP) and the meaning of the features cited later in this sentence, which is definitely beyond the scope of this report, it seems important to point out that the use of object-oriented programming constructs, which actually enhance flexibility, modularity and reuse of software, all nice things, require the compiler to use virtual methods calls, dynamic dispatching, and so on. All these operations are resource intensive and in some cases, they can heavily affect the code performance, and this becomes evident in applications in which such use is done thousand times every simulation step. Even if compiler technology and

implementation solutions are progressing rapidly to overcome the problems by enhancing dynamic code generation (e.g. Richter, 2005; Duffy, 2005; Golding, 2005; Pobar, 2005; Erisman 2006), the problem is not about re-designing or re-factoring software; instead, it is about the general strategy to follow. Be aware that we do not mean that such features should not be used, instead it addresses that using them at run-time is very costly. In other terms, the full use of OOP in the phase of building applications based on biophysical models is an extremely valuable resource, as it is to extend applications and to provide an effective architecture of applications themselves, but it probably should be minimized for use of biophysically based models at run-time. An alternative option is introduced in the next paragraph.

The second option to overcome the problems deriving from modelling framework architecture and use, as defined in the previous page, is far more interesting and can be very effective also with respect to other desirable features in a modelling system, such as complete transparency (the ability of a model to be a self-documenting construct), reproducibility, and verification of models as components of scientific argumentation (Muetzelfeldt and Massheder, 2003). It involves defining models declaratively (as opposed to imperative implementation given by coding), using for instance as declarative language a dedicated definition based of the extended mark-up language (XML), and then producing platform- and framework-specific implementation of either single components or even of the whole simulation system. Making reference to the discussion at the end of the previous paragraph, code generation in this case allows optimizing code, using the less expensive, more direct options to link both models being implemented and existing libraries. In fact, appropriateness of links, matching of types, all is done during the phase of model building, hence it is not needed to "keep alive" resource-intensive mechanisms to allow both for flexibility and extensibility in the phase of model building at run-time, that is when such mechanisms are not needed anymore. The modelling environments Simile (Muetzelfeldt and Massheder, 2003) and Modelica (http://www.modelica.org/) are examples of such architectures to move from model building to operational use. Modern platforms (.NET and Java) provide extremely powerful features for code generation (e.g the NET namespaces System.Reflection.Emit and System.Codedom).

Visual environment software tools allow the conceptual model to be translated into declarative code. This is very important as it allows the modeller to concentrate on the simulation approach, which is described via a graphical language (or via a language than can be easily visualized with an icon-based approach), rather than forcing the modeller to write code, which will necessarily include dependencies on the functioning of the whole simulation system. The use of visual modelling tools, which allows a formal description of models, is by definition cross-language and cross-platform because it provides a standard description of the model that can be easily and automatically translated into different computer languages. Finally, the visual approach allows the development of models and simulation systems that are auto-documented. However, as yet there are only the first prototypes of software that allows, to some extent, switching between textual and graphical representations of a model. These have not yet found favour among model developers, except in principle. The reasons are in part due to habits and in part to functionalities, for instance related to the use of arrays, which can be fairly simply managed using an imperative language (for developers used to coding) but are rather more difficult to handle in a visual representation. Furthermore, it has not yet been clarified how to deal with debugging.

What has emerged in the first 18 month of the project, opposite to past experience when implementation has often being the most challenging task, is that the major effort is thinking in "modular", "multiple choices", modelling terms. Elaborating on model modularization will have positive consequences also on implementations different than the one used in the prototype 1, to the extent of being a sound foundation also for making models available using

a declarative language. The use of declarative modelling is one of the key methodologies chosen for SEAMLESS, and it is consequently a goal to develop the infrastructure needed to make a full operational use of it. This is the priority for the prototype 2 in terms of software implementation, as partial development of the set of tools needed will not allow operational use of declarative modelling, and will not convince modellers to use the declarative modelling implementation paradigm.

# 2 The library of components

Components, as defined in the introduction, are discrete software units to be used for composition, hence, components cannot be used in isolation. The interface that a component makes available and the steps to follow to use it, all consequences of its design and implementation, are then of primary importance for its use. Further, the reason for adopting a component-based paradigm for implementing models as computer programs is to achieve specific functionalities not available with monolithic structures. Consequently, component architecture and implementation are crucial in developing a component base system for biophysical simulation.

The modelling domain of each component and the subdivision of the modelling system in sub-systems are presented in the following figure, where the main components of APES are shown. To meet the requirements of the system (see 2.1.1) a finer granularity was sometimes chosen, i.e. by subdividing a component into more than one discrete software unit.
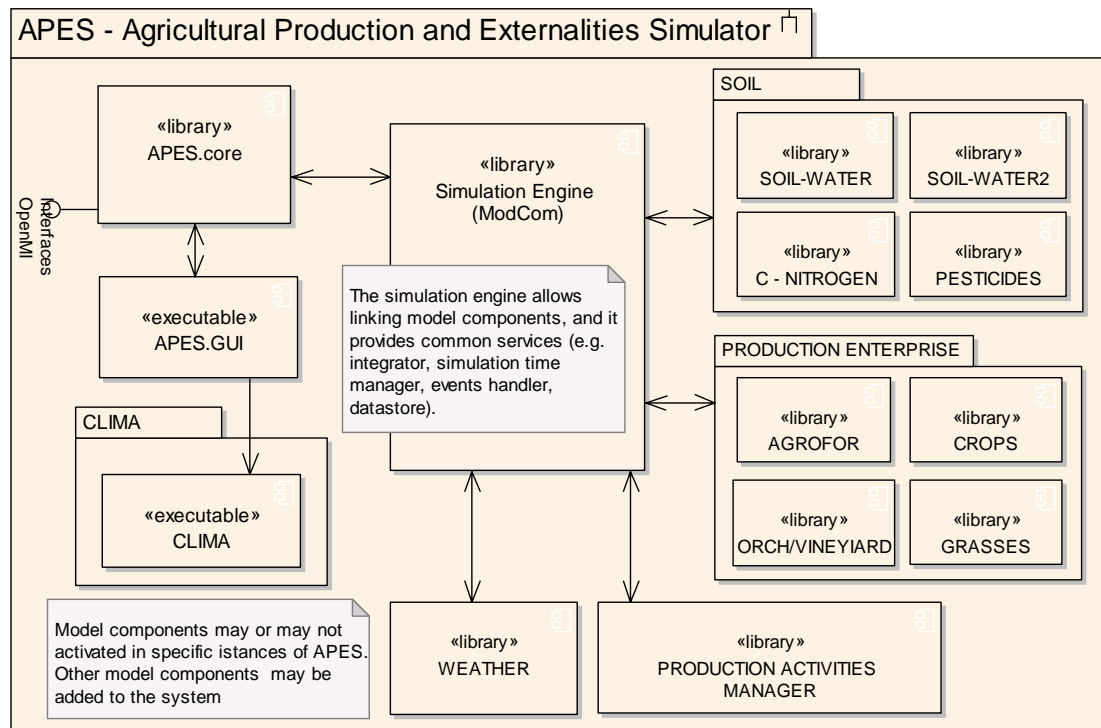
**Fig. 1** *APES component diagram. APES is composed of three main groups of software units: the graphical user interface and the core services component to run Modcom; the simulation engine Modcom, and the model components. Model components can be grouped as soil components, production enterprise components, weather and agricultural management. Note that an alternate option for simulating soil water (SOIL WATER 2) is being developed to provide a first test for components replaceability.*

Several criteria have driven the selection of a sub-set of components for prototype 1, starting from time constraints, which forced to concentrate on a subset of actions to maximize chances to match the deadline. Such criteria can be grouped as 1) due to simulation input/output needs, and 2) due to technical needs. Such criteria are listed below.

1) Criteria due to simulation input/output needs. In SeamFrame, APES is linked to the Production Enterprise Generator, the Production Technique Generator, and the Technical Coefficients Generator (see deliverable 3-2-19). More specifically, the former two provide inputs to APES, whereas the latter uses its outputs. The three generators mention are also under development and needed to test a basic set of inputs (to be supplied to APES) and outputs (to be received from APES). Further, the test cases analyses planned for the first prototypes also required some specific outputs to be transformed in indicators and to be used in the analysis. Consequently, components selection was driven by the need of:

- Make available simulation water and nitrogen limited production;

- Make available simulation of processes which lead to main possible externalities of the system: soil erosion, runoff, nitrogen dynamics in the soil, agrochemicals fate;

- Make available the simulation event driven of agricultural management;

- Test links from components beyond the technical aspect, that is, testing the process of building a consistent input-output matrix and using semantically rich interfaces;

- Have concrete realizations to discuss criteria for model selection within component and then component matching

- Provide an articulated example of parameter needs

- Provide an articulated example of models implemented to derive abstractions for model testing, thus leading to designing proper tools for the purpose

2) Criteria due to technical needs. Whether the abstractions and general concepts of a modelling framework are consolidated, moving from simple proofs of concept to actual, articulated applications needs to be tested and worked out not only with respect to implementation details, but also testing aspects related to multi-team work. The criteria for selecting components for prototype 1 consequently were:

- Implement various components to test different types of connections: for instance, all components are connected to agro-management and weather, agro-chemicals and soil carbon-nitrogen needs soil water, crop should be able to run, for potential production, with the weather component only, soil water might be able to simulate a bare soil with the weather components only;

- Link different components from the point of view of matching inputs-outputs from the technical point (e.g. arrays, units) and at various times during simulation (across and within time steps);

- Implement "one per type", meaning including a crop component (grasses / vineyards / orchards / agroforestry will basically fill the same "slot"), a soil water component (components replaceability will be tested using soil water 2), a soil carbon and nitrogen component, an agro-chemicals component, an agro-management component, a weather component, in order to start:

  o Building proper graphical user interfaces (e.g. to show soil profiles for water, nitrogen, agro-chemicals outputs; to test agricultural management configurations input and output);

  o Testing input/output procedures (access to input sources, various forms of simulation outputs persistence)

  o Testing system performance (ease of model building and execution time)

- Provide articulated samples to allow designing and testing of the relevant part of the knowledge base

- Evaluate the impact of using relatively new IT technologies with teams with different expertise

Within components, beyond what stated in the introduction, a mandatory criteria for model selection is that single models must be peer reviewed to build the foundation of confidence not only in APES, but also in the content of the knowledge base to be built. Developing a component for a specific domain could also be seen as making a review of modelling approaches available as peer reviewed sources, and make them available also for use by third parties. If a new modelling approach is needed because no peer reviewed model is available for a specific purpose, the modellers involved in the project may develop new approaches, in this case submitting a paper to review.

The following section presents the architecture (section 2.1) of the components currently available (section 2.2) as first prototypes, while a third section (section 2.3) presents other components being developed, some already used in the current APES release, others to be included in the coming releases.

## 2.1  Component architecture

### 2.1.1  Component requirements

The solution of biophysical modelling problems can be implemented with different designs and different technologies. Developing a design and selecting a technology should be the result of a careful definition of requirements. The requirements below were defined for model components:

**Functional requirements**

- Estimate/generation of variables via different models;

- Estimate parameters from observational data;

- Provide data at run time, accessing either observational or generated data, and making available model outputs;

- Provide quality checks on data imported;

- Provide quality checks on outputs produced;

**Non-functional requirements**

- Ease of use: the components must be usable by clients easily: impact on technology and on documentation;

- Extensibility: the capability of easily adding alternate processing capabilities to the ones of the component from the side of the component user, without needing to recompile the component, and using the same interface;

- Reusability: the practical possibility of using the component in different software systems; ease of use and solution to a common modelling problem are the keywords;

- Replaceability: the capability of being replaced by a different component respecting the same contract. "Different" here means either a newer version of the same component, or an implementation from a different party;

- Documentation: models, software design, code;

- Unit tests: units tests for each public method, input-output tests reported on documentation.

**Technological requirements**

- Language: C# (.NET platform);

- Documentation: HTML-style, PDF.

## 2.1.2  Ontology

The components contain information extracted from a public ontology.  Information consist of concepts  (variables in this case, which can be seen as instances of the concepts) and of several attributes for each variable, encapsulated using the VarInfo type available in the Preconditions component (see 2.2.5). The description of the VarInfo type follows, with some comments:

- **varName**: the name chosen for a variable. The variable name uniquely identifies the variable with its scope.  Note that the naming convention used, although sometimes not correct with respect to English, is used to keep similar/related variables close in lists ranked alphabetically.  For instance, instead of extraterrestrialRadiation and hourlyExtraterrestrialRadiation, we called the variables  extraterrestrialRadiation and extraterrestrialRadiationHourly.

- **description**: the information to complement what might not be unequivocally understandable from meaningful variable names.

- **default value**: a default value assigned to the variable. This is used to set up initial conditions (when applicable), or to provide a value for parameters (parameters will have the same metadata structure).

- **minValue, maxValue**: minimum and maximum values attached to the variable. They are used to restrict the range of variability (in order to prevent the client from using unreasonable values) and perform pre- and post condition tests. Note that a variable may be estimated from other variables via a model. In this case, the minValue and maxValue of the latter variables allows the range of the derived variable to be computed.

- **units, varType**: units and enumeration types. They are used to link components to the simulation engine, and in case of the units, to perform consistency checks.

Among these attributes the properties with respect to data flow are not included as they are not an intrinsic attribute of the variable. In other words, a variable can be an input in a model, and an output in another model.

The use of this information is in the domain classes described below. The components also contain internal information about parameters and variables, using the same VarInfo type. Such information is defined in the component and used as described in the paragraph pre post conditions).

The information above was used to populate a shared ontology, which is implemented in the project as a web based application available at:
http://seamless.idsia.ch/seamontology/chooser/chooser.php?page=Variables

A model interface is defined as a collection of variable definitions. Collections of variables that are associated with particular domains define the Domain Classes (e.g. we could define the *SoilDomainClass* as the collection of all measurements that are measured on Soil). Such collections can be manually entered by a user or they can be automatically built, using the built-in reasoning features of an ontology. The definition of domain classes in the component

interface allows abstracting the dependency of the model from the data and fostering the extensibility of models via design patterns.

Having defined a domain class in the ontology, an OWL file can be parsed to generate the source code of the model interface or the domain class respectively. An application to generate C# code of domain classes has been developed (Domain Class Coder, http://craisci.icamodelling.it/dcc/). Using domain classes, a modeler can exploit the knowledge structured in the ontology in different modeling frameworks or different programming languages. The adoption of an ontology-driven approach for defining a model interface has clear advantages as it enables the reusability of models in a more easy way, while common problems related to poor semantics of model interfaces can be effectively tackled. Currently, the APES ontology is being populated.

### 2.1.3   Components design

Different designs have being used in the first, exploratory development of components for APES, basically limiting the requirements to the use of a .NET language (all have used C#). The reason was to facilitate as much as possible the development of the first release of APES by taking advantage of work that had already been carried out for a different purpose. The design traits summarized in this paragraph have been adopted, with small differences, in the components described in 2.2.

The general requirement meant to be realized via the design choices made was to produce intrinsically reusable components, that is not targeted specifically to a given modelling framework. To be truly reusable a component must have limited dependencies, be fully documented, and require a modest effort to be re-used. More capabilities could have been obtained, say by making a large use of inheritance; instead, the design chosen makes use of interfaces which specify what a class or the component must do, not how. This increases flexibility which in turn favors replaceability. Also, components are "light-weight": they do not carry dependencies to whole frameworks to be used. The specific design choices made are briefly discussed in the following paragraphs.

### 2.1.3.1   Model granularity

A model can be defined as a conceptualization of a process. This is one possible definition of a model, relevant to the work of developing components for biophysical simulation. A model can be implemented in a class, providing the estimation/generation of a variable (or a set of interrelated variables), obtaining a fine level of granularity. There might be more than one way to estimate/generate a variable.  If two different models estimate variable A, those two models are alternatives to estimate variable A even if they have different input requirements and different parameters. As a consequence, the two models must be available as separate units, and their input, parameters and output must be defined. Such units are here called "strategies", from the related design pattern introduced below.

A way to have available in a component all models, via the same call, including alternate approaches, is the implementation of the design pattern Strategy (Mesketer, 2004). The design pattern Strategy offers the user of the component different algorithms by encapsulating them in a class called Context. Different algorithms, which are alternative options to do the same thing, are called, as introduced above, strategies. When building a biophysical model component this allows in principle to offer alternate options to estimate a variable or, more in general, to model a process. This often needed feature in the implementation of biophysical models, if implemented using the design pattern Strategy, comes with two very welcomed benefits from the software side: 1) it allows an easier maintenance of the component, by facilitating adding other algorithms, 2) it allows to add easily further algorithms from the client side, without the need for recompiling the

component, but keeping the same interface and the same call. The basic point here is that a strategy (a model class) encapsulates a model, the ontology of its parameters, and the test of its pre/post conditions (see 2.1.3.3). It can be used either directly as a strategy (in this case we call it "simple strategy", where simple indicates that is does not use other strategies as part of its implementation), or it can be used as a *unit of composition*, as described below.

A composite strategy differs from a simple strategy because it needs other (simple) strategies to provide its output(s). A sequence of calls might be implemented inside a composite class. The list of inputs is given but includes all the inputs of all classes involved (except those which are matched internally). The list of outputs includes all outputs produced by each strategy and the ones specific of the composite class (if any). The list of parameters needed includes the ones of the classes associated and the ones (if any) defined in the composite class; when the value of a parameter is set, if the parameter belongs to an associated class, it is set on that class. The test of pre/post conditions makes use of the methods available in each simple strategy class associated, plus the new tests specified in the composite class. If a violation of pre/post condition occurs in one of the associated classes, the message informs not only about the violation occurred, but also in what class occurred. Composite strategies do not differ in their use compared to simple strategies. An example of simple and composite strategies is given by Villa et al. (2006). Composite strategies too can be added to the components without requiring a re-compilation of their code, thus providing a way to extend component models in full autonomy by third parties. Composite strategies are solutions to modelling problems at a coarser granularity (in principle) with respect to simple strategies. As an example, a composite strategy may be built to simulate "crop potential production" and be developed composing simple strategies such as "light interception", "crop development", "leaf area expansion", etc. In other terms, a composite strategy is a "closed" solution which makes use of selected models of finer granularity as units of composition (simple strategies, see previous paragraph). Such a closed solution is not meant to be proposed as the unique solution for a specific modelling problem. Making reference to the example above about "crop potential production" two composite strategies may use different simple strategies to simulate "light interception" if they target the simulation of either homogeneous canopies or wide-row spacing crops. Whether such diversity in light interception models might not cause noticeable differences in outputs when simulating potential yield, it may lead to sharp differences when simulating water-limited production in arid environments. Further, two alternate approaches to model light interception say for "homogeneous canopies" could be implemented in two composite strategies, and this would allow for comparison of modelling approaches at fine granularity. This kind of composite models will provide a sound foundation to select modeling approaches to be used at operational level.

The formalization of models in basic units of composition (simple strategies) and in aggregated units (composite strategies), providing the same interface, and decoupling interfaces and data from modelling equation as discussed in the next paragraph, provides the design infrastructure to link and populate a knowledge base. The use of semantically rich interfaces fosters safe reusability of components as discussed in the introduction. Finally, simple and composite strategies are discrete units of code which can be directly used either to build components, or even "full" simulation models to be used stand alone, in the latter case still preserving the benefits of a modular system as described in the introduction.

### 2.1.3.2 Decoupling implementation of interfaces and data from model equations

Targeting model component design to match a specific interface requested by a modelling framework decreases its reusability. This can partly explain why modeling frameworks,

although in theory a great advance with respect to traditional model code development, are rarely adopted by groups other than the ones developing them.

A possible way to overcome this problem is to adopt a component design which targets intrinsic reusability and interchangeability of model components (e.g. Donatelli et al., 2004; Donatelli et al., 2005). This may lead, in the worst cases, to the need for a wrapper class (specific to a modeling framework) as proposed by the Adapter pattern (Gamma et al. 1994) that makes possible the migration to other modelling frameworks.

A key design criterion, which enhances reusability and interchangeability, and which allows concurrent development of both components and clients, is separating the model equation component interface and its implementations, in different software units (D'Souza and Wills, 1999; Cheeseman and Daniels, 2000; Löwy, 2003). Self-standing interfaces decouple clients and providers. This is known as the Bridge pattern (Gamma et al., 1994; Mesketer, 2004) and it allows defining *units of reusability* (model component implementations and model component interfaces) and *units of interchangeability* (model component implementations alone).

In practical terms related to component development in APES, specifying data-structures (domain classes) for different domains via a shared ontology allows concurrent development of the components which will use their own domain classes and other from other components as parameters in their interface. Once the specific software units with data structures and interfaces are implemented, linking and replacing components can be much simpler (Rizzoli et al., 2005). Such separation is implemented in the AgroManagement, AgrochemicalsFate, SoilWater, and SoilErosionRunoff components (see section 2.2). When the SoilWater2 component (see section 2.3) is available, it will be possible to replace SoilWater with SoilWater2 without requiring any change in other components.

### 2.1.3.3   Common features of model components

Model components share a set of features to minimize the effort needed to learn how to use them, and to take advantage of common features. For instance, the application Model Component Explorer (see 2.1.4) allows discovering interfaces, domain classes, inputs etc. because of the above mentioned common features.

**Pre and post conditions tests**

Implementing the test of pre- and post-conditions is the central idea of the Design-by-Contract approach (DBC). In DBC software, entities have obligations to other entities based upon formalized rules between them. A functional specification, or 'contract', is created for each module. Program execution is then viewed as the interaction between the various modules as bound by these contracts. In general, routines have explicit preconditions that the caller must satisfy before calling the routine, and explicit post-conditions that describe the conditions that the routine will guarantee to be true after the routine finishes. When implementing biophysical models, the implementation of the DBC approach not only ensures the correct functionality of the software, but it also specifies what are the limits of use of our model, which is knowledge about the model itself. Also, it allows data of uncertain quality to be used: if an input (either an exogenous variable or the output of another component) is out of the range expected, an exception can be fired, both informing the user of the problem and allowing for exception handling. The DBC approach is implemented via a utility component developed for the purpose, called Preconditions (see 2.2.6).

**Unit tests**

In computer programming, a unit test is a procedure used to verify a particular module of source code is working properly. The idea about unit tests is to write test cases for all

functions and methods so that whenever a change causes a regression, it can be quickly identified and fixed. The goal of unit testing is to isolate each part of the program and show that the individual parts are correct. Unit testing provides a strict, written contract that the piece of code must satisfy. Beyond the general benefits which derive from unit tests, implementation in software development, implementing unit tests to test model implementation and making available the relevant input-outputs in the documentation allows the user of the components to have sample application results for the specific model.

**Models and software design & use documentation**

Each component has a HTML-style help which contains detailed documentation about the models implemented, and information about the design and use of the component. The documentation provided allows re-implementation of all the models of the component, although the characteristics of reusability of the component make it much easier to use, rather than to duplicate it. Another HTML-style file made available for each component is the code documentation, following the standard of the MSDN - .NET documentation.

**Exception handling**

Exception handling is a programming language construct designed to handle runtime errors or other problems (exceptions) which occur during the execution of a computer program. Handling exceptions is of crucial importance in a component based system as it prevents the system from crashing and it allows users (the applications / subsystems using the components) to know precisely the source of the error. Components handle exceptions and provide a custom message informing users which component and class are the source of the error.

**Maximize API ease of use**

One of the key elements for component adoption by third parties is the simplicity of default usage cases via the  application public interface (API). The usage model for component-oriented design follows a pattern of instantiating a type (a class) with a default or relatively simple constructor,  setting some instance properties, and finally, calling some simple instance method. This is called the Create-Set-Call pattern (Cwalina and Abrams, 2006), and it has been implemented in the components. Source code examples for components use provided show example of such usage.

## 2.1.4   Discovering component and model interfaces

The Model Component Explorer (MCE http://craisci.icamodelling.it/mce/) is a Windows application to inspect model components to discover interfaces, domain classes, VarInfo values, simple and composite strategies, and their parameters, inputs and outputs.

Taking as an example the assembly CRA.clima.et.interfaces.dll in Fig. 2, ETData is a Domain Class and ETDataVarInfo is the relevant VarInfo class. All model strategies are available in the component CRA.clima.et.dll. Currently, not all components can be explored using the MCE).

The interface and the domain classes are discovered by selecting an assembly via the button Discover Interfaces. The screen image of Fig. 2 shows also the content of the Domain Class. Note that by clicking on a property in the list, the VarInfo attributes are shown.

By selecting a model component via the button Discover Strategy, all the strategies are shown, and all outputs produced by the component are also listed. Selecting a strategy causes the display of the relevant parameters, inputs, and outputs. If an output is selected on the list right to the list of the strategies, in the list box below all the strategies (one or more) which produce that output are shown (Fig. 3).

If a composite strategy is selected (a composite strategy is associated with other strategies), the associated strategies are shown. If the list box associated strategies is empty, that means that the strategy being inspected is a simple strategy. If a parameter is selected, its VarInfo values are shown
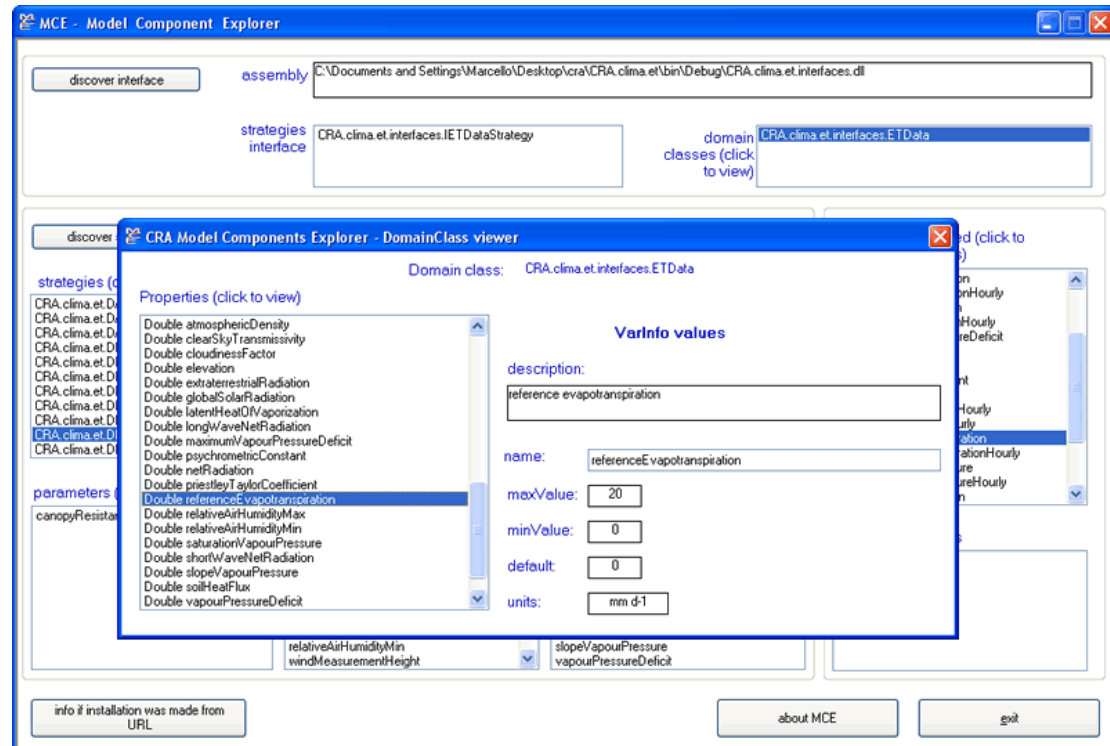


**Fig. 2** *Inspecting domain classes and VarInfo values of a component via the Model Component Explorer.*
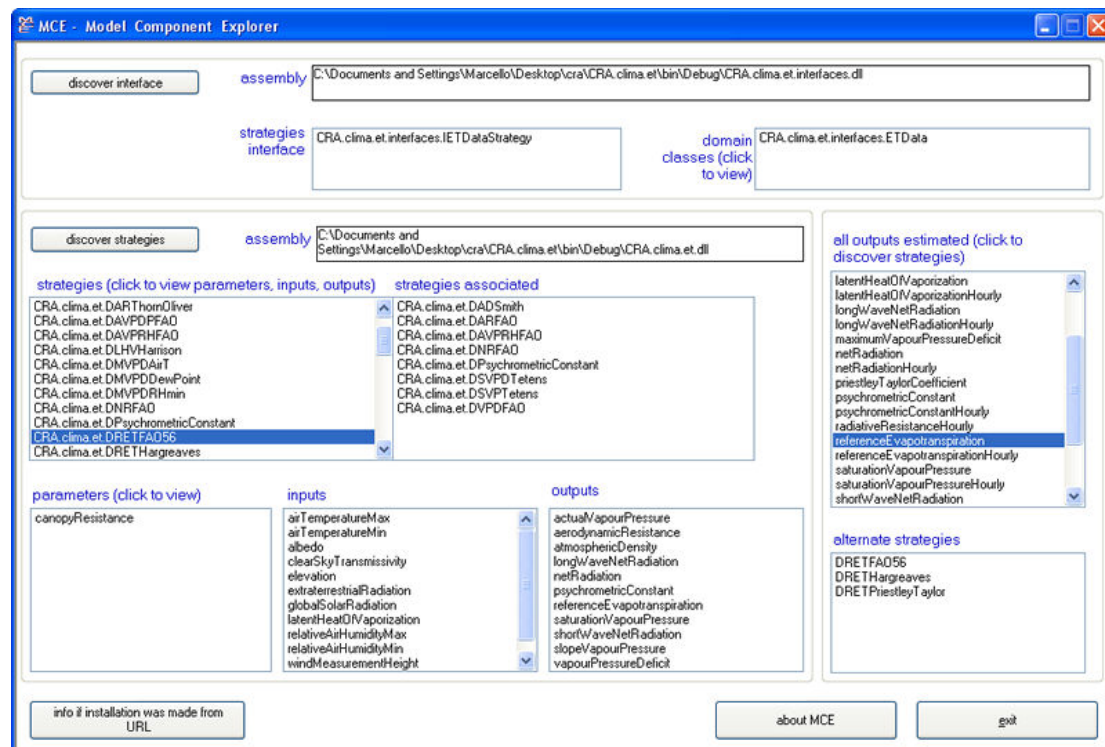
**Fig. 3** *Discovering strategies in a model component via the Model Component Explorer. DREFAO56 is a composite strategy which is built using the simple strategies listed in the box "strategies associated" (see 2.1.3.1 for details).*

## 2.2 Components available

Components available for download include dynamic link libraries, help and code documentation, and source code examples for their use. They are all available for free download via web as specified in appendix B.

All model components implement a dependency to the "impact" data structures of the component AgroManagement (see the following paragraph) to be able to recognize published agro-management events, thus being able to implement the relevant impact.

The following paragraphs contain summaries of the models implemented in the components. Full documentation is available in the PDF version of the help files provided, and it includes the relevant references which are not reported in following summaries to avoid duplication.

### 2.2.1 AgroManagement

The AgroManagement component is designed to implement production management actions within the system. An agricultural activity is defined, in this context, as a production enterprise (e.g. a crop rotation, an orchard) associated with a production technique (e.g. irrigated, high nitrogen fertilization, minimum tillage). Such an integrated system must be implemented in a way that imitates as closely as possible farmers' behaviour. Limiting the drivers of the decision making process to the biophysical system implies that each action must be triggered at run time via a set of rules, which can be based on the state of the system, on constraints of resources availability, or on the physical characteristics of the system. However, simulating management in a component-based system poses challenges in defining a framework which must be reusable and able to account for a variety of agricultural

management technologies applied to different enterprises. Finally, the implementation of management must allow using different approaches to model its impact on different model components.
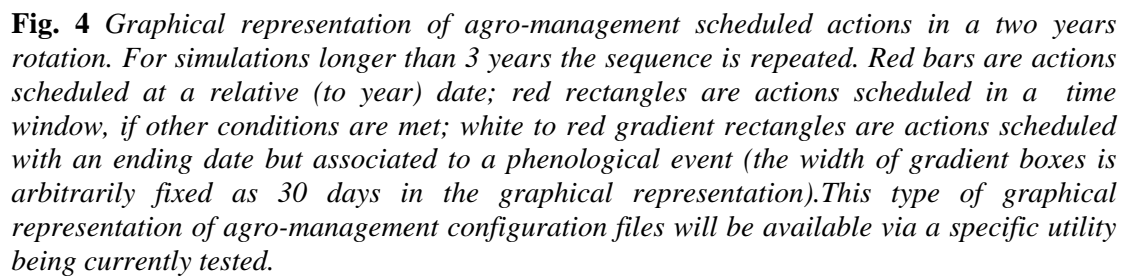
The AgroManagement component formalizes the decision making process via models called rules, and it formalizes the drivers of the implementation of the impact on the biophysical system via set of parameters encapsulated in data-types called impacts. Each operation must have a rule to be applied at run time; when the rule is satisfied, a set of parameters is made available to model components for the implementation of the impact. The component is easily extendable for both rules (which have the structure of strategies, hence rules encapsulate the attributes for each parameter, allow for testing of pre-conditions, and use the same interface implemented to allow the extensibility of the component) and impacts, so that the use of the AgroManagement component allows different modelling approaches to be used. Furthermore, the information on the biophysical system is passed via a data-type called states, which can also be extended. This is important as the current data-type includes the information needed by the rules currently implemented; newly implemented rules might require further variables which can then be added. The output (in terms of management actions to be applied as resulting from rules evaluated at run-time) drivers, to provide a simulation output (e.g. to output to a text file, to an XML file, and to a database, all currently available) can be fully customized by the user as well by adding new ones without recompiling the component.

The rule-based model is characterized by 3 main sections:

- Inputs: states and time

- Parameters (values are compared to rules via the rule model)

- A model which returns a true/false output

Rules can be based on relative date or based on a set of state variables and are implemented as a class encapsulating its parameters declaration and test of pre-conditions (this also allows management configuration files to be validated via pre-condition tests).

Parameters are needed by model components to implement the impact of management. There are few parameters which are common to a generic management event (e.g. management type) and to a specific management event (e.g. water amount for irrigation, tillage depth for tillage). Other parameters (are needed by specific management approaches (e.g. implement type can be needed by a specific approach to model tillage, as opposed to other approaches to model tillage which do not need such information) and generally at least partially differ even within specific management event types. An example of graphical representation of a management configuration, for a two- years rotation, is shown in the figure below.

**Fig. 4** *Graphical representation of agro-management scheduled actions in a two years rotation. For simulations longer than 3 years the sequence is repeated. Red bars are actions scheduled at a relative (to year) date; red rectangles are actions scheduled in a time window, if other conditions are met; white to red gradient rectangles are actions scheduled with an ending date but associated to a phenological event (the width of gradient boxes is arbitrarily fixed as 30 days in the graphical representation).This type of graphical representation of agro-management configuration files will be available via a specific utility being currently tested.*

The following table shows the VarInfo attributes of inputs in the use of the component in the release APES v 0.3; rule and impacts parameters are detailed in the documentation and provided via an XML file. Not all dates of phenological events are used in the current version of APES, but the current structure allows for synchronizing management to detail phenological models.

Table 1 *AgroManagement inputs (implementation in APES v 0.3).*

| name | units | maxValue | minValue | defaultValue | description |
|------|-------|----------|----------|--------------|-------------|
| bulkDensity | t/m3 | 2 | 0.8 | 1.3 | soil bulk density |
| layerThickness | m | 2 | 0.01 | 0.1 | soil layer thickness |
| fieldCapacityVolSWC | m3/m3 | 0.48 | 0.05 | 0.3 | volumetric soil water content at field capacity |
| wiltPointVolSWC | m3/m3 | 0.3 | 0.01 | 0.15 | volumetric soil water content at permanent wilting point |
| soilWaterContentVol | m3/m3 | 0.5 | 0.01 | 0.3 | volumetric soil water content |
| leafAreaIndex | m2/m2 | 15 | 0 | 3 | area of leaves per unit area of soil |
| aboveGroundBiomass | t/ha | 40 | 0 | 1 | above ground biomass |
| airTemperatureAverage | C | 40 | -20 | 10 | average air temperature |
| datePlanting | d | 365 | 0 | 90 | date of planting |
| dateEmergence | d | 365 | 0 | 95 | date of emergence |
| dateFiveLeaves | d | 365 | 0 | 120 | date of five leaves fully formed |
| dateEndJuvanilePhase | d | 365 | 0 | 180 | date of end of juvanile phase |
| dateHeading | d | 365 | 0 | 212 | date of head emission |
| dateBeginTillering | d | 365 | 0 | 190 | date when tillering begins |
| dateTuberRootInitiation | d | 365 | 0 | 200 | date when tuber formation begins |
| EndPhotoInductivePhase | d | 365 | 0 | 212 | date when photo-inductive phase ends |
| BeginStemElongation | d | 365 | 0 | 190 | date when stem elongation begins |
| BeginFlowering | d | 365 | 0 | 210 | date when flowering begins |
| dateBeginGrainFilling | d | 365 | 0 | 240 | date when grain filling begins |
| dateMilkDough | d | 365 | 0 | 240 | date when millk stage occurs in cereals |
| dateSoftDough | d | 365 | 0 | 220 | date when soft dough stage occurs in cereals |
| datePhysiologicalMaturity | d | 365 | 0 | 345 | date of physiological maturity |

## 2.2.2 AgroChemicalsFate

The AgroChemicalsFate component predicts the fate of agrochemicals in the environment. The model considers 5 compartments where pesticide is stored: canopy surface, plant, available fraction of the soil, aged fraction of the soil and bound fraction of the soil, even though it is possible by strategies to exclude the bound and aged fractions. The available fraction is partitioned in 3 phases: gas, liquid, and solid.

Models are implemented in four composite strategies:

- Air
- Crop
- Canopy
- Soil

The "air" models consider the processes that occur before the pesticide reaches the soil, and they simulate the processes of drift and plant interception.
The differentiation between the virtual compartments "crop" and "canopy" is related to the different processes simulated: on "canopy" the agrochemicals are subject to transformation and can mobilize, whereas "crop" is a sink of agrochemicals. Neither toxicity of accumulated chemicals on the plant, nor the impact on plant products quality, is estimated.
From the surface, the chemical may enter the soil system, transported by infiltrating water and is partitioned among the gas, liquid and solid phases of the soil. The soil compartment is divided in two parts, the first represents the process over the soil surface, the second describes the soil profile. Chemicals are degraded in the soil profile by chemical, photochemical and microbial processes and might be taken up by plant roots.

The component has to be linked to other components to run and to describe the behaviour of pesticides in the modelled system. It is well known that the main determinant of pesticide flow through the soil profile is advection. It is necessary, therefore, that the component reads information about water content and water fluxes from the soil water component. Soil has to provide also temperature because several processes are affected by it. The crop strategy

requires information about the crop, in particular about ground cover to estimate crop interception of pesticides during application.

The following tables show the VarInfo attributes of inputs and outputs in the use of the component in the release APES v 0.3.

Table 2 *AgrochemicalFate inputs (implementation in APES v 0.3)*

| name | units | maxValue | minValue | defaultValue | description |
|---|---|---|---|---|---|
| FieldArea | m2 | 1.79769313 | 0 | 0 | Surface of the field |
| FieldPerimeter | m | 1.79769313 | 0 | 0 | Field perimeter |
| LAI | dimensionless | 1.79769313 | 0 | 0 | Leaf area index |
| Rain | m d-1 | 1.79769313 | 0 | 0 | Amount of rain |
| WaterLeaching | m d-1 | 1.79769313 | 0 | 0 | water flux out the bottom |
| WaterRunOff | m d-1 | 1.79769313 | 0 | 0 | runoff volume |
| BulkDensity | t m-3 | 1.79769313 | 0 | 0 | Bulk density |
| CarbonOrganic | % | 100 | 0 | 1 | Organic carbon |
| LayerThickness | m | 1.79769313 | 0 | 0 | Layer thickness |
| WaterFraction | dimensionless | 1.79769313 | 0 | 0 | water content fraction |
| WaterFractionFieldCapacit | dimensionless | 1.79769313 | 0 | 0 | water content at field capacity |
| WaterFractionSaturation | dimensionless | 1.79769313 | 0 | 0 | water content at saturation |
| WaterLayerFlux | m d-1 | 1.79769313 | 0 | 0 | Flux of water from upper layer |
| WaterRootUptake | m d-1 | 1.79769313 | 0 | 0 | Water root uptake |

Table 3 *AgrochemicalFate outputs (implementation in APES v 0.3)*

| name | units | maxValue | minValue | defaultValue | description |
|---|---|---|---|---|---|
| DayAfterApplication | d | 1.7976931348 | -1.797693134 | 0 | day after the last application |
| Available2DrainTotal | g m-2 d-1 | 1000 | 0 | 0.1 | total flux of pesticide from available fraction to drain sy |
| Available2Leaching | g m-2 d-1 | 10 | 0 | 0.1 | flux of pesticide to leaching |
| Available2TransformedTotal | g m-2 d-1 | 1000 | 0 | 0.1 | total flux of pesticide from available fraction to transfor |
| Canopy2Transformed | g m-2 d-1 | 10 | 0 | 0.1 | flux of pesticide that transform on the canopy |
| DriftLoss | g m-2 | 10 | 0 | 0.05 | drift loss |
| PesticideOnCanopyState | g m-2 | 10 | 0 | 0 | amount of pesticide on the canopy |
| PesticideOnPlantState | g m-2 | 10 | 0 | 0 | amount of pesticide in the plant |
| VolatilizedTotal | g m-2 d-1 | 10 | 0 | 0.1 | total flux of pesticide to volatilized (from canopy and fr |
| Available2RunOff | g m-2 d-1 | 10 | 0 | 0.1 | flux of pesticide from available fraction to runoff |
| Available2Volatilised | g m-2 d-1 | 10 | 0 | 0.1 | flux of pesticide from available fraction to volatilised |
| Available2Drain | g m-2 d-1 | 10 | 0 | 0.1 | flux of pesticide from available fraction to drain system |
| Available2Transformed | g m-2 d-1 | 10 | 0 | 0.1 | flux of pesticide from available fraction to transformed |
| SoilContent | g m-2 | 1000 | 0 | 0.005 | Concentration in available, aged and bound fractions |
| LiquidFlux | g m-2 d-1 | 10 | 0 | 0.1 | pesticide flux in liquid phase |
| PesticideAgedState | g m-2 | 10 | 0 | 0 | amount of pesticide in the Aged fraction |
| PesticideAvailableState | g m-2 | 10 | 0 | 0 | Pesticide concentration in available phase |
| PesticideBoundState | g m-2 | 10 | 0 | 0 | amount of pesticide in the bound fraction |

### 2.2.3 SoilWater and SoilErosionRunoff

The SoilWater component describes the infiltration and redistribution of water among soil layers, the changes of water content, fluxes among layers, the effective plant transpiration and soil evaporation, and the drainage if pipe drains are present. Two algorithms have been selected to simulate the water dynamics, a cascading algorithm and a cascading with travel time among layers. The cascading method simulates the soil as a sequence of tanks that have a maximum and a minimum level of water, fixed respectively at the field capacity (FC) and wilting point (WP). Water in excess of the water content at FC for a given layer is routed into the lower layer, and if all the profile has reached FC, the water in excess is removed from the soil as percolation. The main advantage of this approach is the simplicity and the calculation speed. The main difficulties are that the model has not a strong physical background, because the concept of field capacity is a practical approximation and represents a simplification of soil water holding features, and because the time needed to water to move between layers is not considered. Other relevant difficulties of this approach is the impossibility to have soil

water contents greater than FC and lower than WP (the latter with exception of the evaporative layer), and the possibility to have allowed movement of water only downwards. This approach is not suitable where there are layers of different texture or a water table, even if it is possible to use some approximation to simulate the capillary rise. The cascading method with travel time is an extension of the simple cascading method, taking into account the time needed to percolate the layer. Tillage simulation is done following the approach of the models Wepp and SWAT, where each type of equipment used on the soil has specific parameters and a coefficient for the intensity of tillage (mixing among layers), for surface roughness after tillage, ridge high and distance This allows for the simulation of the evolution of bulk density in time, because a simple model of soil settling after tillage was also developed. Currently, all the variables are simulated with a daily time step, but the algorithms and software structure are ready to work with an hourly or shorter time step.

The SoilErosionRunoff component simulates dynamically water runoff and soil erosion. In detail, it represents the runoff volume, the amount of soil eroded, the interception by vegetation, and the water available for infiltration. This component has been structured in a hierarchical way with the above-described Water component, but has its own data-type and related interfaces. As for the Water component, all the variables are simulated using a daily time step, but the algorithms and software structure are already designed to work with an hourly or shorter time step.

The following tables show the VarInfo attributes of inputs and outputs in the use of the component in the release APES v 0.3.

Table 4 *SoilWater/ErosionRunoff inputs (implementation in APES v 0.3)*

| name | units | maxValue | minValue | defaultValue | description |
|---|---|---|---|---|---|
| EvaporationAttainable | mm / d | 15 | 0 | 0.5 | Attainable evaporation from the upper soil layer. |
| FieldSlope | 0 - 1 | 0.3 | 0 | 0.05 | Field slope |
| Lai | m / m | 12 | 0 | 0 | Leaf area index |
| Rain | mm / d | 500 | 0 | 0 | Rain |
| RootBiomass | t / ha | 20000 | 0 | 5 | Root biomass |
| ReferenceDrainageDepth | m | 100 | 0 | 0 | Reference Drainage Depth |
| RootDepth | m | 1.5 | 0 | 0 | Depth of roots in the soil profile. |
| TranspirationAttainable | mm / d | 15 | 0 | 0 | Attainable transpiration |

Table 5 *SoilWater/ErosionRunoff outputs (implementation in APES v 0.3)*

| name | units | maxValue | minValue | defaultValue | description |
|---|---|---|---|---|---|
| Drainage | mm / d | 100 | 0 | 0 | Amount of drained water |
| Erosion | t / ha d | 50 | 0 | 0 | Amount of soil eroded |
| EvaporationActual | mm / d | 15 | 0 | 0.5 | Actual evaporation from the upper soil layer. |
| FieldLength | m | 500 | 1 | 100 | Field length |
| FieldWidth | m | 500 | 1 | 100 | Field width |
| CropInterception | mm / d | 500 | 0 | 0 | Rain intercepted by crop |
| TranspirationActual | mm / d | 15 | 0 | 0 | Actual transpiration |
| Runoff | mm / d | 300 | 0 | 0 | Runoff in the time step of one day |
| BulkDensity | t m-3 | 1.8 | 0.9 | 1.3 | Bulk density |
| OrganicCarbon | % | 100 | 0 | 1 | Organic carbon |
| SaturatedHydraulicConductivity | mm h-1 | 1800 | 0.1 | 50 | Saturated hydraulic conductivity |
| Thickness | m | 3 | 0.05 | 0.05 | Soil layer thickness |
| VanGenuchtenAlpha | cm-1 | 0.1 | 0.003 | 0.02 | Alpha variable of VanGenuchten's hydraulic retention |
| VanGenuchtenN | dimensionless | 5 | 0.5 | 2 | N variable of VanGenuchten's hydraulic retention func |
| VolumetricFieldCapacity | m3m-3 | 0.7 | 0.03 | 0.3 | Field capacity |
| VolumetricWaterContent | m3m-3 | 0.8 | 0 | 0.2 | SoilWaterContent |
| VolumetricWaterContentAtSaturation | m3m-3 | 0.8 | 0.32 | 0.45 | soil water content at saturation |
| VolumetricWiltingPoint | m3m-3 | 0.4 | 0.01 | 0.1 | Volumetric water content at wilting point |
| WaterFlux | mm d-1 | 1000 | -30 | 0 | The amount of water that drains from a soil layer to a |
| WaterPotential | kPa | 10000 | -2 | 33 | Soil water potential |

### 2.2.4  Weather

Weather components implement several strategies, from peer reviewed sources, to estimate variables subdivided in five domains. Emphasis is placed in sharing and making available for operational use modelling knowledge produced by research. Weather components can be considered as a realization of a part of "Numerical recipes in agro-ecology" as proposed by Leffelaar et al. (2003), implemented using an updated technology. The reason for the subdivision in components is to make it easier to re-use and maintain the models. The reference to the peer reviewed sources of the models is available in the documentation.

### 2.2.4.1  AirTemperaure

The generation of daily maximum (Tmax, °C) and minimum (Tmin, °C) air temperatures is considered to be a continuous stochastic process with daily means and standard deviations, possibly conditioned by the precipitation status of the day (wet or dry). Three alternative methods are implemented for generating daily values of Tmax and Tmin, all based on the assumption that air temperature generation is a weakly stationary process. The multi-stage generation system is conditioned on the precipitation status with two approaches. Residuals for Tmax and Tmin are computed first, than daily values are generated - independently (Richardson-type) or with dependence of Tmax on Tmin (Danuso-type). A third stage, that adds an annual trend calculated from the Fourier series, is included in Danuso-type generation. Another approach even accounts for air temperature-global solar radiation correlation. A third approach generates Tmax and Tmin independently in two stages (daily mean air temperature generation first, Tmax and Tmin next), making use of an auto-regressive process from mean air temperatures and solar radiation parameters. Daily values of Tmax and Tmin are used to generate hourly air temperature values, according to alternative methods. Sinusoidal functions are largely used to represent the daily pattern of air temperature. Six approaches, are used to generate hourly values from daily maximum and minimum temperatures. A further approach derives hourly air temperatures from the daily solar radiation cycle. Mean daily values of dew point are estimated via empirical relationships with Tmax and Tmin and other variables. A diurnal pattern (hourly time step) of dew point is also modelled via two alternative methods.

### 2.2.4.2  Evapotranspiration

Evapotranspiration for a reference crop (ET0) is calculated from alternative sets of inputs and for different canopies, conditions and time steps, using one-dimensional equations based on aerodynamic theory and energy balance. A standardized form of the Penman-Monteith equation is used to estimate daily or hourly ET0 for two reference surfaces. According to FAO Irrigation and Drainage Paper n. 56, the reference surface is a 0.12-m height (short crop), cool-season extensive grass such as perennial ryegrass or tall fescue . A second reference surface, recommended by the American Society of Civil Engineers, is given by a crop with an approximate height of 0.50 m (tall crop), similar to alfalfa. The Priestley-Taylor equation is useful for the calculation of daily ET0 for conditions where weather inputs for the aerodynamic term (relative humidity, wind speed) are unavailable. The aerodynamic term of the Penman-Monteith equation is replaced by a dimensionless empirical multiplier. As an alternative when solar radiation data are missing, daily ET0 can be estimated using the Hargreaves equation. An adjusted version of this equation, according to Allen et al. is given. Stanghellini revised the Penman-Monteith model to represent conditions in greenhouse, where air velocities are typically low ($<1.0$ m s$^{-1}$). A multi-layer canopy is considered to estimate hourly ET0, using a well-developed tomato crop, grown in a single glass, Venlo-type greenhouse with hot-water pipe heating. The Stanghellini model includes calculations of the solar radiation heat flux derived from the empirical characteristics of short wave and long

wave radiation absorption in a multi-layer canopy. A leaf area index is used to account for energy exchange from multiple layers of leaves on greenhouse plants. The constituent equations of the Stanghellini model are in accordance with the standards of the American Society of Agricultural Engineers.

### 2.2.4.3  Rain

The occurrence of wet or dry days is considered to be a stochastic process, represented by a first-order Markov chain as described by Nicks et al. The transition from one state (dry or wet) to the other (dry or wet) is governed by transition probabilities, as characterized monthly by analyzing historic long-term daily precipitation data for the site. According to the multi-transition model of Srikanthan and Chiew, the daily precipitation amounts are divided into up to seven states - dry or wet from 1 (lowest rainfall) to 6 (highest rainfall). On days when precipitation is determined to occur the precipitation amount is generated by sampling from alternative probability distribution functions. Most approaches are based on the two-state transition model for dry/wet days. The Gamma distribution is used to model precipitation amounts for the last state (highest level of rainfall) in the multi-state transition probability matrix of Srikanthan and Chiew, while a linear distribution is applied for the other states. The pattern of Gamma plus linear distribution across various occurrence states exhibits a combined J shaped function.

Short-time rainfall data are generated by disaggregating daily rainfall into a number of discrete events, then deriving the characteristics (amount, duration and starting time) for each event. Four approaches have been implemented to disaggregate daily rainfall into six hour or shorter periods (as small as 10 minutes). The method described by Arnold and Williams uses a 0.5-hour time resolution and assumes that daily rainfall falls in only one event. The peak location is generated first according to a broken linear distribution. The other 0.5-hourly amounts are generated from an exponential distribution and relocated on both sides of the peak. The other methods are more flexible and able to capture bursts of storm occurring discontinuously over the day. In the approach by Meteoset an autoregressive process and a Gaussian daily profile model are combined to simulate the possibility of precipitation at any hour. Two options are available to generate sub-daily precipitation events for varying time steps. The cascade-based disaggregation method of Olsson breaks each time interval into two equally sized sub-intervals. The total amount is redistributed into two quantities according to two multiplicative weights from a uniform distribution: 24-hour rain into two 12-hour amounts, 12-hour amount into 6-hour amounts, and so on until 1.5-hour resolution is achieved. The approach by Connolly et al. allows disaggregation of daily rainfall into multiple events on a day, and the simulation of time-varying intensity within each event: (1) distinct storms are assumed independent random variables from a Poisson distribution, (2) the storm origins arrive according to a beta distribution, (3) storms terminate after a time that is simulated by a simplified gamma distribution, (4) each storm intensity is a random value exponentially distributed, (5) time from the beginning of the event to peak intensity is given by an exponential function, (6) peak storm intensity for each event is also determined from an exponential function, (7) internal storm intensities are represented by a double exponential function.

### 2.2.4.4  SolarRadiation

Solar radiation outside the earth's atmosphere is calculated at any hour using routines derived from the solar geometry. Daily values are an integration of hourly values from sunrise to sunset. The upper bound for the transmission of global radiation through the earth's atmosphere (i.e., under conditions of cloudless sky), can be set to a site-specific constant or estimated daily by diverse methods.

Broadband global solar radiation (about 0.3-3.0 μm wave-band) striking daily horizontal earth's surfaces is estimated from alternative sets of weather inputs according to strategies based on either physical relationships or stochastic procedures. A sine-curve is used to deduce the hourly distribution of solar radiation from its daily value, assuming changes with solar elevation angle. The most simplified models relate diurnal temperature range to solar energy transmission through the earth's atmosphere. Since one of the most important phenomena limiting solar radiation at the earth's surface is cloudiness, a cloud cover measure is incorporated in the model from Supit and van Kappel to estimate transmissivity. The radiation model from Winslow et al. uses saturation vapour pressures at minimum and maximum air temperature as a measure of the atmospheric transmission of incident solar radiation. The Ángström and Prescott model is the most common choice to estimate global solar radiation when sunshine measurements are available. As an alternative, an implementation of the model of Johnson et al. and Woodward et al. is given. Stochastic generation is based on the dependence structure of daily maximum and minimum temperature, and solar radiation. Such variables are reduced to time series of normally distributed residual elements with mean zero and variance of one. An autoregressive, weakly stationary multivariate process is used to generate the residuals. Daily values of global solar radiation are generated for dry and wet days as daily deviations above and below the monthly average value. An implementation by Garcia y Garcia and Hoogenboom is given as well.

The flux density on a horizontal plane at the earth's surface is comprised of a fraction of direct beam, coming directly from the direction of the sun, and diffuse radiation coming from many directions simultaneously. The irradiance on a tilted surface includes the fraction reflected from the ground calculated from a slope-dependent factor. The current implementation for a tilted surface derives from the general approach from Liu and Jordan. The estimation of diffuse radiation on a horizontal surface depends on the extra-terrestrial irradiance and a transmission function. Hourly transmission relies on the assumption of anisotropy for estimation on inclined surfaces and is further divided into the isotropic, circumsolar and horizontal ribbon sub-fractions. These sub-fractions are calculated separately and then summed to provide the diffuse irradiance. The direct fraction of solar radiation is the complement to diffuse solar radiation. The visible band (0.38-0.71 μm wavelength) is estimated daily by the diffuse/direct radiation ratio, and hourly by the solar elevation course. PAR amount can be also disaggregated into direct and diffuse fractions. Slope is the angle the surface makes with the horizontal plane, and aspect is the clockwise orientation to south. One or both are required to compute geometric factors that convert radiation estimates from horizontal to non-horizontal surfaces. An ESRI-based approach is implemented to derive slope and aspect from digital elevation data grids.

### 2.2.4.5 Wind

Daily mean values of windspeed, are generated by sampling from alternative probability distribution functions. Following generation of daily mean wind speed, alternative approaches are available to estimate the maximum and minimum wind speeds for the day. Like most climatic variables, windspeed tends to be both random and cyclic as time varies. Probability distribution functions are used to randomly distribute daily mean wind speed within the day. Alternatively, wave functions are used to describe average diurnal wind speed variations using reference values of both maximum and minimum wind speeds for the day as inputs.

### 2.2.4.6 ClimReader

Crop, cropping system and hydrological models at field level often require meteorological data at daily or hourly time resolution. Such data may include a range of variables (e.g.

maximum and minimum daily air temperature, daily rainfall, daily evapotranspiration). Meteorological data also require site-specific data (e.g. latitude, clear sky transmissivity). CRA.ClimReader.dll is a component which allows loading location and provides meteorological data at run-time. It also loads the soil data, which also need to be loaded at the start of the run. The component allows loading of data in different formats (txt, XML, and from MS Access), and different sets of data, allowing for flexibility of data sources. Missing data are often a feature of meteorological records. The component allows estimation of some meteorological variables if missing in the input file: reference evapotranspiration, vapour pressure deficit, day length, global solar radiation. Reference evapotranspiration can be estimated using the Hargreaves, Priestley-Taylor, and Penman-Monteith method according to data availability. The component uses ET, AirT, Wind, Rain, and GSRad components.

Table 6 *ClimReader outputs (implementation in APES v 0.3)*

| name | units | maxValue | minValue | defaultValue | description |
|---|---|---|---|---|---|
| airTemperatureMax | °C | 50 | -10 | 15 | daily maximum air temperature |
| airTemperatureMin | °C | 35 | -25 | 5 | daily minimum air temperature |
| airTemperatureDailyAverage | °C | 43 | -17 | 15 | average of maximum and minimum air temperature |
| albedo | unitless | 0.9 | 0.05 | 0.2 | ratio between reflected and incoming radiation |
| angleSlope | degree | 90 | 0 | 0 | surface inclination angle respect to an horizontal surface |
| angleAspect | degree | 359 | 0 | 0 | clock-wise orientation angle to South |
| clearSkyTransmissivity | unitless | 0.85 | 0.52 | 0.75 | fraction of clear sky global solar radiation at ground level |
| globalSolarRadiation | MJ m-2 d-1 | 38 | 0.01 | 20 | daily global solar radiation at ground level |
| latitude | degree | 90 | -90 | 45 | latitude of the site |
| rain | mm d-1 | 400 | 0 | 20 | daily precipitation amount |
| referenceEvapotranspiration | mm d-1 | 20 | 0 | 0 | reference evapotranspiration |
| vapourPressureDeficit | kPa | 12.31 | 0 | 1 | vapour pressure deficit |
| windSpeed | m s-1 | 100 | 0 | 1 | wind speed |

## 2.2.5 Preconditions

Preconditions is a utility used by all the model components described above. This component facilitates the testing of pre- and post-conditions, and contains the definition of the VarInfo type. The component Preconditions is currently used in the components AgroManagement, SoilWater, SoilErosionRunoff, AgrochemicalsFate, AirTemperature, Evapotranpiration, Rain, SolarRadiation, and Wind. This component also contains the definition of other interfaces which are used in all components. Several pre- and post conditions can be tested at each call. Pre-conditions which can be tested as variables values are:

- variable values within a range (VarInfo maxValue e minValue),

- one value lower than another,

- at least one value of a matrix different from zero,

- if one value has a value different from zero another value cannot be zero,

- if a value is in a range, another value must be in a given range.

Using the range test, at least two types of custom specifications can be made in a class:

1) the range of a variable of the domain class can be narrowed to match the ones of the model being implemented: a VarInfo variable is defined, then the new minValue and maxValue are set, and finally the current value of the domain class variable is assigned as current value, on which the test is made

2) custom tests for composite variables can be made by defining a range in class (e.g. a VarInfo variable is defined say as siltPlusSand, then the minValue and maxValue are set), then the current value to be tested at each time step is set as the sum of sand + silt values, thus defining a composite value.

Pre- and post-condition tests can have a output to the screen, to a text file, or to a XML file, and using custom format which can be developed implementing an interface of the component. The output format is a strategy, and a strategy implemented by a client does not require the recompilation of Preconditions, as described for model components.

## 2.3 Components under development

Model components already implemented in version .0.3 of APES, but still under development include Crops (2.3.1) and SoilCarbon-Nitrogen (2.3.4). Such model components are available as Modcom classes and are not available as independent software units. Other components, not included via APES in the first SEAMLESS-IF prototype are under development, i.e. those for Grasses, Vineyards and Orchards, SoilWater2 and Agroforestry.

### 2.3.1 Crops

The LINTUL model has been implemented in the current framework to simulate biomass production as a function of intercepted radiation and its conversion efficiency. The crop growth is limited by two factors, the water stress and the nitrogen limitation. Water stress is modelled via the ratio between actual and potential transpiration; when a water stress event occurs, the simulated crop allocates more biomass to the roots and less to the shoot which increases the potential access to soil water. The simulation of nitrogen stress follows the growth dilution concept as implemented in the crop model CropSyst. Radiation use efficiency is reduced by a fraction when the available percentage of nitrogen is between the minimum nitrogen requirement and the critical nitrogen requirement.

The crop model is linked to nitrogen turnover assuming that roots take up the required nitrogen over the whole soil profile implying that only one dynamic soil layer needs to be considered. The Soil Carbon-Nitrogen component, uses the layering of soil horizons done by the Soil Water component into a number of discrete fixed layers. Therefore, given a certain depth of the roots, a demand of attainable nitrogen uptake is passed to the Soil Carbon-Nitrogen component, receiving, before integration, the actual uptake.

The model reacts also to the irrigation and fertilization regime, including soil nitrogen mineralization, which depends on soil temperature. Since the susceptibility of crops to water and nitrogen availability depends on crop development stage, the impact of different management strategies could be investigated by the model.

The current model assumes that pests, diseases, weeds and pollutants are non-limiting so that the crop does not suffer any adverse impact. Phenology depends on temperature, the crop will reach full maturity and ready to be harvested at a certain temperature sum, but the harvest itself will usually take place somewhat later. Possible losses between these dates are not accounted for in the current model. At harvest either the whole of the crop or only crop compartments may be taken from the field. The parts of the crop that remain on the field after harvest will be used as an input to the soil organic matter module.

The LINTUL model was written in the simulation language FST, Fortran Simulation Translator. The Fortran code containing the rate equations, which is generated by FST, is encapsulated in a Fortran dynamic link library. The version used in APES, version 0.3, was written using C# as a Modcom class, which accesses crop parameter values from an XML file.

Future development of the crop component will aim at decoupling the different model processes to implement models using a finer granularity, thus allowing the user to create, combine and assess different modelling approaches.

Table 7 *Crop inputs (implementation in APES v 0.3)*

| name | units | maxValue | minValue | defaultValue | description |
|---|---|---|---|---|---|
| GlobalSolarRadiation | MJm-2d-1 | 40 | 0.1 | 20 | daily global solar radiation |
| AirTemperatureMin | C | 35 | -5 | 15 | Daily minimum air temperature |
| AirTemperatureMax | C | 45 | -2 | 15 | Dailymaximum air temperature |
| PotentialEvapotranspiration | mm.d-1 | 20 | 0 | 8 | Potential Evapotranspiration |
| ActualTranspiration | mm.d-1 | 20 | 0 | 8 | Daily actual plant transpiration |
| PlantNitrogenUptake | gN.m-2d-1 | 1 | 0 | 0.5 | Daily actual plant nitrogen uptake |

Table 8 *Crop outputs (implementation in APES v 0.3)*

| name | units | maxValue | minValue | defaultValue | description |
|---|---|---|---|---|---|
| AirTemperatureSum | Cd | 3000 | 0 | 1110 | Accumulation of daily average air temperature from emerg |
| LeafAreaIndex | m2.m-2 | 20 | 0.01 | 3 | Leaf area index |
| WeightGreenLeaves | g.m-2 | 500 | 0 | 100 | Weight of green leaves |
| WeightDeadLeaves | g.m-2 | 500 | 0 | 100 | Weight of dead leaves |
| WeightStems | g.m-2 | 1000 | 0 | 500 | Weight of stems |
| WeightRoots | g.m-2 | 100 | 0 | 30 | Weight of roots |
| WeightStorageOrgans | g.m-2 | 2000 | 0 | 800 | Weight of storage organs |
| RootDepth | m | 2 | 0.1 | 0.5 | Rooting depth |
| DevelopmentStage | unitless | 2 | 0 | 1 | Stage of development of the plant |
| AmountNitrogenRoots | gN.m-2 | 2 | 0 | 1 | Nitrogen amounts in roots |
| AmountNitrogenStorageOrgans | gN.m-2 | 20 | 0 | 10 | Nitrogen amounts in storage organs |
| AmountNitrogenLeaves | gN.m-2 | 10 | 0 | 5 | Nitrogen amounts in leaves |
| CNratioLeaves | unitless | 30 | 0 | 15 | CN ratio of leaves |
| CNratioStems | unitless | 100 | 0 | 50 | CN ratio of stems |
| PotentialTranspiration | mm.d-1 | 20 | 0 | 8 | Potential transpiration of plant |
| Ndemand | gN.m-2d-1 | 1 | 0 | 0.5 | Total nitrogen demand of the plant |

### 2.3.2 Grasses

The grassland model needs to simulate biomass accumulation for a wide range of grasses species and react dynamically to management practices, such as defoliation and fertilization. Thus, we chose as a basis the biophysical sub-model of SEPATOU developed by Cros et al., which simulates herbage growth under a range of different management strategies.

This model was extended to a large range of grass species by including the concept of plant functional type, based on a typology developed within INRA, Toulouse. These plant functional types are defined according to grassland utilisation (grazing, cutting) and sward nutrient status (defined through fertilization and plant available nitrogen, given by the soil component). Therefore, such definition of criteria allows (1) predicting herbage accumulation rate under different management practices and (2) evaluating the impact of these practices on biomass production. Plant functional types group species according to their common responses to the environment (response trait) and/or common effects on ecosystem processes (effect trait). Therefore, inclusion of this concept into the grass model by defining specific parameters applicable to multi-species grassland made the model generic and therefore applicable at the European level.

The model includes simulation of: light interception, biomass growth via radiation use efficiency, senescence and remobilization, biomass partitioning, water and nitrogen uptake.

The grass model was developed to simulate permanent grasslands. However, it can be extended to temporary grasslands by considering them as Plant Functional Type A or B, depending on their attributes, especially for phenology. These plant functional types are defined according to grassland utilisation (grazing, cutting) and sward nutrient status (defining through fertilization and plant available nitrogen, given by the soil component). Therefore, such definition of criteria allows (1) predicting herbage accumulation rate under different management practices and (2) evaluating the impact of these practices on biomass production. However, the approach does not consider (1) extensive rangelands, (2) summer pasturing (in mountainous regions) and (3) fallows. Furthermore, the model was developed

from the perspective of simulating grassland production from North to South of Europe with a good sensitivity to management practices and climatic differences within a specific zone.

To determine thermal time within the model and consequently phenological variables such as leaf life span, average daily temperatures outside the range from 0 to 18°C were set to these limit values. As climatic conditions deviate more from those considered when the model was created, e.g. in the Baltic or Mediterranean regions, there may be a need for some recalibration of the model. Threshold values may need to be re-evaluated for more extreme conditions, usually leading to the presence of other graminea or dicotyledons from the ones considered within the typology of Cruz et al.

Finally, the primary goal of the implemented model within the grassland component was to establish impact of management on grassland production for specific regions. Although up-scaling the model to the European level may lead to some discrepancies in taking into account weather variability (as mentioned previously), it should still be effective for considering the impact of management practices.

The grassland model is implemented as a "one-model per class" (one strategy) and directly inherits methods from ModCom, hence using C# as development language.

### 2.3.3   Vineyards and Orchards

Modelling orchards are very specifics to one species and even if theoretically, formalisms can be extended to every woody perennial crop. It will require an additional work of calibration to adopt a common way of modelling grapevine and apple tree growth for instance. For the time being, we dispose of two different versions of the component, one for modelling grapevine and another for apple tree. The grapevine component version dated from month 15 and has not been changed since this date whereas the Apple component is most recent (month 18) and differs in some points. At this stage of development we adopted and validated in priority modelling approaches described in the literature and validated. However, even if tests are being performed on different parts of the model, the whole component has not been validated yet with field data.

The components are able to simulate:

- yield, average sugar and water content of the product, and the time-course of biomass production in leaves, branches and fruits [general outputs] + Biomass of roots and trunk, Mean single fruit fresh weight [Apple outputs];

- the harvest and winter cane pruning [main management events] (only stand-alone version);

- the biomass of senesced leaves and pruned stems [outputs for soil components];

- potential transpiration, potential soil evaporation and root length distribution throughout the profile. [outputs for soil components].

Climate data and information about the layout of the plot are required to compute the potential production of the annual aboveground biomass. A computation of a water and nitrogen stress index is in progress to allow the linkage with the soil components.

To reach the first objective, namely to provide a prototype version of the fruit tree component running under the Modcom environment, several assumptions/simplifications were made:

- only mature trees (i.e. with a standard architecture) are simulated;

- the soil surface is considered as bare and only one species is growing on the plot;

- only the annual aboveground organ production is taken into account; that is to say leaves, stems and fruits [Grapevine];

- the biomass is allocated to the different organs of the crop using look-up tables;

- the inter-annual impact of carbon storage is neglected;

- the product quality is described by the water content and the sugar content of fruits + Mean fruit fresh weight [Apple];

- root length growth is driven by soil temperature and is disconnected from the biomass production [Grapevine].

The model calculates the annual growth of grapevine aboveground biomass (fruits, leaves, stems); some quality variables such as fruit sugar content and fresh weight are also estimated. To allow the future linking with soil components, the root length growth and its distribution throughout the soil profile is also calculated as well as the potential transpiration and evaporation.

Even if for many points orchards and vineyards can be simulated the same way, discrepancies between them exist due to the specificity of orchard management or to physiological behaviours of fruit trees closer to forest trees. Because apple production is the most important fruit production in Europe, the Apple tree has been chosen as the species to be simulated in the APES orchard component. Modelling apple tree orchards required some predictable adjustments and the actual version contains three innovations compare to the vineyard version. The growth concerns the annual and the perennial part of the tree that allows the coupling between the root growth procedure and the computation of the root distribution in the soil. The calculation of the mean weight of a single fruit has also been added, this variable is closely related to the fruit grade that determines the price of the product. The procedure of calculation makes use of an external input, the fruit load, that has to be defined by the user. As shown in numerous studies the fruit load affects greatly the global production of biomass and the allocation of carbon in the different organs. Theses two major effects are also simulated by the model.

At present, the model does not cope with an environment with a limiting supply of water and nutrients. Impacts of water and nitrogen shortage on growth will be integrated in the forthcoming version. For the second prototype, once the software structure will be satisfactory enough, more efforts will be put in testing and improving the concepts to reach the objective of modeling the growth of two species (grapevine or fruit tree, and intercrop) concurrently on a single plot.

Most recent developments have dealt with the development of a wrapper and domain classes to achieve the functionalities provided by the modular design of APES. Such modifications aimed at improving re-use, interchangeability and extensibility of the software unit.

The component has been developed in C# to facilitate its integration into the Modcom environment. In parallel a stand-alone model has been written in FST (Fortran Simulation Translator) to test different algorithms.

### 2.3.4   Soil Carbon-Nitrogen

The nitrogen and carbon dynamics are described in the routines of the Soil Carbon-Nitrogen component, of which the SUNDIAL model forms the basis. This model simulates all of the major processes of C and N turnover in the soil/plant system using only simple input data. This feature makes this model an ideal choice to be implemented as base for the C and N modelling in the current framework. In SUNDIAL, the microbial processes of carbon and

nitrogen turnover are described together with mineralization and immobilisation occurring during decomposition of soil organic matter. Furthermore, the bypass flow following addition of fertiliser, the nitrification of ammonium to nitrate, and the nitrogen losses by denitrification are also represented in detail. In synthesis, therefore, the model should:

- simulate microbial and physical processes influencing the C and N content of the soil, greenhouse gas emissions and leaching losses from the soil;

- allow addition of C and N to the soil as crop residues, organic manures, fertilisers and atmospheric deposition using information supplied by other components;

- use input information about the soil water and temperature provided by other components to simulate the microbial and physical processes of C and N turnover and loss;

- output the distribution of mineral N down the soil profile, so that other components can determine the availability of N to a plant root at a given depth;

- output the nature of losses of C and N from the system so that pollution events can be investigated.

The SUNDIAL soil C and N routines have been modularised so that they are separated from crop, water and cultivation routines. The initialisation, addition, microbial and physical processes are distinct in the new code. A C# version of the code has been completed as a Modcom class and included in release 0.3 of APES.

### 2.3.5   Soil Water 2

Soil Water 2 represents in detail the water dynamics within the soil profile. It differs from SoilWater (see 2.2.1) mostly in that it accounts for preferential water flow in the soil profile. The soil structure is a matrix of solid phase holding water and air on several smaller scales. The module simulates dynamics of both soil structure and soil-water interacting together.

The profile consists of a surface layer and 4 underlying horizons. The surface layer can reproduce the impact of technical practices as tillage or effect of a crust on water infiltration and evaporation where surface hydraulic conductivity, layer thickness and maximum surface storage are the three principal modified factors. Each horizon is a pedostructure, a homogeneous zone in term of structure and organisation. The soil is discretized into 10 layers. To preserve a modelling logic between layers and horizons, the depth of each layer is determined by the model using the depth of the horizons provided by the user. The equation used allows the uniformity of the layer's depth in each horizon and differences between horizons. The initial water content of each horizon has to be provided by the user.

A model version in C# has been completed and verification of the code is on going.

### 2.3.6   Agroforestry

The agroforestry component needs to be able to predict both the productivity of agroforestry systems, and some of their environmental impacts. However, agroforestry systems are very diverse as they combine numerous tree species with most major crops of Europe. The simultaneous presence of trees and crops represents the major challenge in simulating agroforestry systems, given also the 1D simplification of other APES components.

Modelling agroforestry implies a need to model competition between trees (usually individual trees) and crop components (usually a population of plants). Competition occurs for all the

resources needed by plants: light, space, water, nitrogen, mineral nutrients. Availability of a below-ground water table plays a key role in such competition.

The tree growth module in APES will dynamically model the tree growth over decades. This module will be generic and could be used for any perennial crop with a canopy (vineyards, orchards, large trees). This dynamic tree component will interact with the crop component competing on resources use. The tree component will be described by an average tree (tree to tree variability will not be described by the model). The tree will have access to an areaof land whose size depends from the tree density in the stand. Modelling perennial plants implies that carbohydrate and nitrogen reserve pools need to be modelled, which make the growth model trickier. These pools are essential for modelling correctly the rapid increase of leaf area after budburst, fruit production, and the reaction of the plant after pruning.

The APES tree module will also include a fruit pool, but the prediction of the fruit yield is considered not attainable with the simple structure of APES. It is therefore suggested that the number of fruits should be introduced as a forcing variable in the APES tree module. The number of fruits that will be forced should take into account any farmer action of fruit number reduction (mechanically or chemically). The tree module will then predict the fate of this pool of fruits, taking into consideration the competition between the various tree sinks for carbon.

C allocation will be governed by two types of rules

- Teleonomic (or goal driven) allocation rules based on allometric equations defining the relative sizes of above-ground sub-compartments and below-ground sub-compartments;

- An optimal allocation assumption ('functional equilibrium') between above ground and below ground mediated through stress indices.

Six structural tree parts are considered

- Stem;

- Branches (distinction between stem and branches is necessary because of alteration of the branch / stem allometry following pruning);

- Foliage;

- Coarse (structural) roots;

- Fine roots (feeder roots);

- Fruits.

Light interception by spaced trees (or rows of vineyards) is a matter of geometry. However, our intention is to maintain a 1D model in APES. A possibility for modelling the light interception by the tree is to take into account the structure of the tree stand (spacing of the trees, shape of the canopies) and calculate the true amount of direct and diffuse radiation that reaches the crop. This means that some aspects of 2D or 3D modelling are introduced in the model, but that these effects are incorporated in parameters of a 1D model. A geometric description of the tree canopies must be done via an appropriate algorithm. This could be the module of the Hi-sAFe model (Dupraz et al, 2004).

Conventional algorithms based on volumetric soil water content or water potential are not able to simulate correctly water competition between different species. This is another case in which the 1D simplification requires strong assumptions. An algorithm that meets the required criteria, and is based on the matrix flux potential can be used simplifying the algorithm in 1D. Water uptake by mono-specific stands at seasonal scale tends to be

dominated by the net supply to the soil (rainfall minus soil evaporation) and evaporative demand (determined by the energy balance), rather than by details of root distribution. This is no longer true in mixed stands.

The implementation of the first prototype of the agroforestry component is on going.

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*SEAMLESS papers* (references about models are included in the documentation of each component, see appendix A)

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# Glossary

| | |
|---|---|
| *Attribute* | A feature within a class that describes a range of values that instances of the class may hold. |
| *Class* | A description of a set of objects that share the same attributes, operations, methods, relationships, and semantics. |
| *Client-server architecture* | In a client-server architecture there is an application (client) which uses a component (server). Client/Server is a scalable architecture, whereby each computer or process is either a client or a server. Although developed as a network application architecture, it is also very effective for component based systems running on local machines. |
| *Component* | A (software) component is a discrete, binary (executable or library - no source code) unit of software. A component is a unit of composition with contractually specified interfaces and explicit context dependencies only. A software component can be deployed independently and is subject by composition by third parties. A component may implement one or more models. |
| *Design pattern* | *A coding solution to implement a given functionality in the code.* |
| *Data-type* | Set of variables grouped to represent a domain (e.g. "soil water") or for a specific use (e.g. parameters to implement the impact on the system of an agro-management action) |
| *Interface* | An interface is a class without implementation. It is thus a specification of behaviour that implementers agree to meet. It is a contract. By implementing an interface, classes are guaranteed to support a required behaviour, which allows the system to treat non-related elements in the same way. |
| *Model* | Conceptualization of a process. This is one possible definition of "model", which is relevant for the work of developing components for biophysical simulation. |
| *Reflection* | Capability in C# (and other languages such as Java) to discover at run time in one assembly (DLL) types (classes), methods, properties, enumerators, allowing also to access their values. |
| *Regression testing* | It is any type of software testing which seeks to uncover regression bugs. Regression bugs occur whenever software functionality that previously worked as desired stops working or no longer works in the same way that was previously planned. Typically regression bugs occur as an unintended consequence of program changes. |
| *Repository* | A repository is a place (or discrete software unit) where data (models) is stored and maintained |
| *Strategy* | Different algorithms which are alternative options to do the same thing can be called strategies. "Strategy" refers to the implementation of an algorithm as a discrete unit of source code |

|  | (a class), implementing a specific interface in order to be used via the relevant design pattern. |
| *Unit of composition* | A unit of source code, namely a class, that can be used to develop composite strategies, that is model classes which require other model classes (of the same component) to produce their output(s). A strategy is a unit of composition. |
| *Unit of interchangeability* | The model component DLL which can be replaced by a different one (either a newer version or a new one) if it respects the contract in the interfaces DLL |
| *Unit of reusability* | The couple of DLLs interfaces and models. |

# Appendix A - Documentation of components

The documentation of models is quite comprehensive. Models are described in the help files which are used to document each of the components; the list below shows the correspondence between components and relevant files. Such files are attached to this report as PDF files, and are also available as compiled HTML-style help files in the components installation installation. The list of downloadable components includes utility components.

- AgroManagement          CRAAgroManagement.pdf

- AgrochemicalsFate         UNICATTAgrochemicalsFate.pdf

- Soil RunOff and Erosion     UNIMISoilErosionRunoff.pdf

- Soil Water                UNIMISoilWater.pdf

- Weather

    - Air temperature     CRAclimaAirT.pdf

    - Evapotranspiration   CRAclimaET.pdf

    - Rainfall               CRA.climaRain.pdf

    - Solar Radiation      CRAclimaGsrad.pdf

    - Wind                 CRAclimaWind.pdf

    - ClimReader        CRAclimaClimaReader.pdf


- Crops                   WURPPSCrop.pdf (*limited to models implemented*)

- Preconditions            CRAcorePreconditions.pdf

# Appendix B – Component availability

| Component | Owner | Download page |
|-----------|-------|---------------|
| SolarRadiation | CRA-ISCI | http://www.sipeaa.it/ASP/ASP2/GSRad.asp |
| Rainfall | CRA-ISCI | http://www.sipeaa.it/ASP/ASP2/Rain.asp |
| Air temperature | CRA-ISCI | http://www.sipeaa.it/ASP/ASP2/AirT.asp |
| Wind | CRA-ISCI | http://www.sipeaa.it/ASP/ASP2/Wind.asp |
| Evapotranspiration | CRA-ISCI | http://www.sipeaa.it/ASP/ASP2/ET.asp |
| ClimReader | CRA-ISCI | http://www.sipeaa.it/ASP/ASP2/ClimReader.asp |
| AgroManagement | CRA-ISCI | http://www.sipeaa.it/ASP/ASP2/AgroManagement.asp |
| SOILWater | UNIMI | http://www.sipeaa.it/ASP/ASP2/SoilWater.asp |
| SOILErosionRunoff | UNIMI | http://www.sipeaa.it/ASP/ASP2/SoilErosion.asp |
| AgrochemicalsFate | UNICATT | http://www.sipeaa.it/ASP/ASP2/Pesticides.asp |
| Preconditions | CRA-ISCI | http://www.sipeaa.it/ASP/ASP2/Preconditions.asp |