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Using Automatic Differentiation to study the sensitivity of a crop model

Lauvernet, C., Hascoët, L., Le Dimet, F.-X., and Baret, F.

Abstract Automatic Differentiation methods are often applied to codes that solve partial differential equations, e.g. in the domains of geophysical sciences, such as meteorology or oceanography, or Computational Fluid Dynamics. In agronomy, the differentiation of crop model has never been performed since the models are not fully deterministic but much more empirical. This study shows the feasability of constructing the adjoint model of a crop model referent in the agronomic community (STICS) with the TAPENADE tool, and the use of this adjoint to perform some robust sensitivity analysis. This aims at giving a return of experience from users working in the environmental thematic, and presents a somewhat unusual field of application of Automatic Differentiation.

Key words: adjoint mode, agronomic crop model, sensitivity analysis

1 Field of application : the agronomic crop model STICS

STICS (Brisson et al, 1998) is a crop model with a daily time-step. Its main aim is to simulate the effects of the physical medium and crop management schedule variations on crop production and environment at the field scale. From the characterization of climate, soil, species and crop management, it computes output variables

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relating to yield in terms of quantity and quality, environment in terms of drainage and nitrate leaching, and to soil characteristics evolution under cropping system[1].

The two key output variables simulated by STICS that we will need in this paper are the Leaf Area Index and the biomass. The Leaf Area Index (LAI) is the total one-sided area of leaf tissue per unit ground surface area (no unit). This is a canopy parameter that allows to directly quantify green vegetation biomass. As the leaves are considered to be the main interfaces with the atmosphere for the transfer of mass and energy (Rosenberg et al. [221]), the LAI indirectly describes properties of the observed surface such as potential of photosynthesis available for primary production, quantification of plant respiration, evapotranspiration and carbon flux between the biosphere and the atmosphere, and gives evidence of severely affected areas (areas burned, attacked by parasites). Because this is the canopy parameter the most observable by remote sensing, the LAI is a very commonly used variable, for example in crop performance prediction during cultivation [5], in models of soil-vegetation-atmosphere [13], in crop models [2, 3], in radiative transfer models for calculating the reflectance [17]. Its values can range from 0 for bare soil to 6-7 for a crop during its life cycle, and up to 15 in extreme cases (tropical forests).

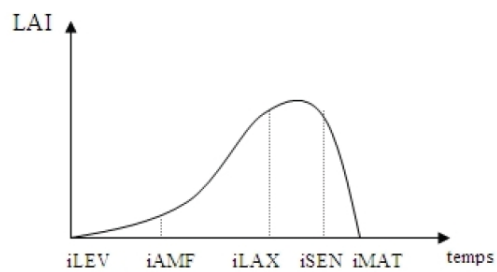

Fig. 1 Simplistic scheme of the stages simulated by the STICS model on dynamics of LAI.

The model STICS simulates the crop growth from sowing to harvest, represented by the evolution of the LAI at selected vegetative stages [2] (Fig. 1). This partly explains the problems to differentiate it described in Sect. 3.2, since it is composed of process threshold. For wheat crop, the main phenological stages are the stage *ear at 1 cm* stage *heading*, stage *flowering*, stage *maturity* (indicated by the water content of the grains). In this work focused on the variable LAI, we are only interested on vegetative stages (LEV, AMF, LAX, SEN), because we do not simulate grain yield but only the total biomass. Stage LEV determines emergence or budding. Stage AMF (maximum acceleration of leaf area index) is the beginning of the elongation of the stem at the end of juvenile growth, and is also called *ear 1 cm*. Stage LAX (maximum LAI) represents the end of leaf growth. Stage SEN is the onset of net senescence.

[1] http://www.avignon.inra.fr/agroclim_stics_eng

2 Sensitivity Analysis

A model is a more or less realistic or biased simplification of the state variable it simulates. This is especially true for agronomic models, since the functioning of vegetation is not *a priori* described by exact equations: agronomic models attempt to predict the behavior of the crop by incremental improvements of the simulation code, based on observations made on the field and then published by specialists. Thus, in some parts of the model, this empirical approach is not based on the equations of some underlying physics or chemistry. Sensitivity analysis, which consists in studying the impact of perturbing the control parameters on the model output allows to understand the model better, improve the quality of the response of the model, and simplify the model.

A sensitivity analysis requires two essential ingredients:

- A model:
$$F(X,K) = 0$$
where X is the state variable (LAI, biomass ...), K are the control variables of the model (parameters θ, forcing variables ...) that the model needs to describe the evolution of X; F is a differential operator *a priori* non-linear finite-dimensional. We assume that for given K, the system has a unique solution $X(K)$. In this study, what we call the model is corresponding exactly to the STICS computer program.
- A response function G which combines one or more outputs of the model into a scalar value, of which one wants to evaluate the sensitivity (for example final value or integral on time of an output).

By definition, the sensitivity of G with respect to K is the gradient of G with respect to X. If we are able to get the adjoint model, the gradient can be computed in only 2 steps: run once the direct model for the value of the parameter in the neighborhood of which the sensitivity analysis is requested, then solve once the adjoint model and the sensitivity is obtained by [10]:

$$\nabla G = \frac{\partial F^t}{\partial K} P$$

where P is the adjoint variable of X. The method of sensitivity analysis using adjoint model is the only one to calculate formally the gradient of the response function and is particularly suitable when the number of entries is large comparing to the size of the response function to analyze [12, 11].

The other sensitivity methods consist in approximating the gradient: finite difference approximation of the gradient require extensive direct model computations, whereas a single run of the adjoint method provides all sensitivities [4]. Stochastic sampling techniques are very intuitive since they consist (roughly speaking) in exploring the space of control to determine an overall (global) sensitivity [15, 8]. These methods have been largely used on the agronomic models and in particular on STICS (e.g. [7, 14, 16]).

If in most of the cases, the response function G is a real function of X, it can happen that the model is driven by threasholds (the code is defined by a lot of branches). Theoretically, a piecewise continuous function is not continuously differentiable, but it has a right derivative and left derivative. The differentiation of such a code does not allow to obtain a gradient of the model but a sub-gradient. In practice, this is not a real problem since the local sensitivty is valid in the vicinity of the points it is evaluated.

3 Automatic Differentiation : application on the STICS crop model

3.1 The TAPENADE Automatic Differentiaton tool

TAPENADE [6] is an Automatic Differentiaton tool based on source transformation. Given a source program written in FORTRAN, TAPENADE builds a new source program that computes the derivatives of the given program. In one mode (tangent mode), TAPENADE builds the program that computes directional derivatives. In a second mode (adjoint mode), TAPENADE builds the program that computes the gradient of the output with respect to all input parameters.

Considering the complete set of derivatives of each output with respect to each input, i.e. the Jacobian matrix of the function computed by the program, the tangent mode yields a column of the Jacobian whereas the adjoint mode yields a row of the matrix. Therefore in our particular case where the output is a scalar G, one run of the adjoint code will return the complete gradient. In contrast, it takes as many runs of the tangent mode as there are inputs to obtain the same gradient. Although we are going to experiment with the two modes, it is clearly the adjoint mode that fits our needs.

However, the adjoint mode needs to evaluate the derivatives in the inverse order of the original program's execution order. This is a tremendous difficulty for large programs such as STICS. The Automatic Differentiation model copes with this difficulty by a combination of storage of intermediate values and duplicated evaluation of the original program, and this has a cost either in memory or in execution time, and generally both. As for the TAPENADE tool, the strategy is essentially based on storage of intermediate values, combined with the storage/recompute tradeoff known as checkpointing that automatically takes place at each procedure call.

3.2 STICS adjoint : the pains and sufferings of an AD end-user

The STICS model being written in FORTRAN 77, it is theoretically possible to calculate its adjoint with the Automatic Differentiation tool TAPENADE. However,

things didn't go so well with the early versions of TAPENADE i.e. before 2005. Later versions brought notable improvements but we believe it is worth describing the main problems that we encountered at these early stages.

Automatic Differentiation allows for instructions which are forbidden by the symbolic differentiation systems. It also provides a real gain in computational time. However, it requires the model to follow some specific hygiene rules to be differentiable: all the input parameters, and especially the "independents", must be clearly identified and if possible separate from the other variables. The same holds for the outputs and especially the "dependents". The precision level of all floating point variables must be coherent, especially for validation purposes: if the chain of computation is not completely "double precision", then the divided differences that is used to validate the analytic derivatives will have poor accuracy, validation will be dubious and may even fail to detect small errors in the differentiated code.

Validation helped us detect small portability problems in STICS. As divided differences requires to call STICS twice, we discovered that two successive calls to STICS apparently with the same inputs gave different results. In fact the first call was different from all the others, which pointed us to a problem of hidden uninitialized remanent global. Fixing this gave us correct divided differences, and a more portable STICS code.

More specifically to this agronomy application, we had problems with the high number of tests and other conditional jumps in an average run. In more classical situations of Scientific Computing, programs are derived from mathematical equations. Typically, they solve a set of ODE's or PDE's. This forces some amount of regularity into the code that discretizes and solves these equations. Even if branches do occur, they rarely introduce discontinuity and the derivative itself often remains continuous. In our application, the program itself basically is the equation. The model evolves by introducing new subcases and subdivisions, i.e. more tests, by hand directly in the source. If, like here in the field of agronomy, this evolution is not made with differentiation in mind then it may introduce sharp discontinuities that do not harm the original code but make it non-differentiable. It took us time to replace faulty branches with a cleaner, differentiable implementation. On the other hand, one can argue that this results in a better code.

Still, the number of branches in the STICS model is very large: thresholds, conditions, loops, and other control all are tests that the adjoint code must remember to run backwards. For these reasons, STICS consumes an unusually large memory to remember this control. Until recently, TAPENADE did not store this control efficiently, using a full INTEGER value to store only a boolean in general.

Chekpointing the time-stepping was difficult. Before binomial checkpointing was introduced in TAPENADE, we had to split the main time loop of 400 iterations into two nested loops of 20 iterations each, and place these two loops into two new subroutines to force checkpointing. We did not have the time at INRA to experiment with the new TAPENADE directives for binomial checkpointing and for checkpointing arbitrary pieces of code, but missing those at the time of our work was a big drawback.

Anticipating on Sect. 3.3, the run time of the adjoint code that gave us the first correct sensitivities is surprisingly slow. This question was put aside for a while, to concentrate on exploiting the sensitivity. The problem has been identified since: it comes from the default checkpointing strategy applied to a chain of 4 nested procedure calls, each of them doing little else than calling the next nested call. As the size of the memory stored by the checkpoint is (inevitably) large, this slowed the code enormously. The answer is to decide not to checkpoint these calls. This finally yields an adjoint code that runs reasonably fast. This also raises the question of finding which procedure calls should be checkpointed and which shouldn't. Support for this is badly missing in TAPENADE.

More than five years after this sensitivity study, both STICS and TAPENADE have evolved. The latest version of STICS model (STICS 6) has been modified, giving a quite more differentiable code than previously. TAPENADE 3.6 had several bugs fixed and more importantly provides a set of user directives to control checkpointing better.

3.3 Validation of the adjoint model

The Taylor test has been performed and converges to 1 for $\alpha = 2^{-16}$, validating the tangent code. The adjoint code was validated by a dot-product test repeated in several directions of perturbation. The times we obtained at the time of the study are:

Direct model : $0.21s$ Tangent model : $0.39s$ Adjoint model : $30.96s$

The run time of the adjoint code is surprisingly slow, 150 times slower than the direct code. We left the problem to the TAPENADE developers to go on with the sensitivity study. The problem was eventually identified, coming from too many checkpoints on procedure calls. This results in the following times, obtained by the TAPENADE team with TAPENADE 3.6:

Direct model : $0.22s$ Tangent model : $0.52s$ Adjoint model : $0.86s$

4 Results : sensitivity analysis of STICS

The adjoint of STICS was calculated in relation to variables of interest (LAI and biomass). The response functions proposed are their integrals on the cycle (up to time T at harvest), in particular to represent the sensitivity of the growth dynamics:

$$G_{LAI} = \sum_{i=1}^{T} LAI(t_i) \qquad G_{biomass} = \sum_{i=1}^{T} biomass(t_i)$$

4.1 Selection of input parameters for sensitivity analysis of output variables

For this feasibility study, the agro-pedo-climatic conditions correspond to wheat crops from the Danube's plain in Romania in 2000-2001 in the frame of the ADAM experiment[2] [1]. The adjoint model was calculated according to the following choices on the input parameters: for LAI, we chose the varietal parameters acting on the dynamics of LAI, and *dlaimaxbrut* that strongly characterizes the aerial growth. Varietal parameters were adapted to the ADAM database in Romania, including the variety of wheat (Flamura) which has particularities towards the cold resistance and phenology. The optimization method used for calibration is the simplex algorithm of Nelder-Mead, which consists in minimizing the gap between simulations and measurements of LAI using a geometric exploration of the space of optimized parameters.

For biomass, efficiencies at three important phases of the cycle of wheat (juvenile phases, vegetative and grain filling) and *vmax2* were chosen following the previous sensitivity analysis combined with the knowledge accumulated by users of the crop model. Table 1 describes the role and the values of these parameters in the vicinity of which the sensitivity was calculated.

Table 1 Parameter role and values in the neighborhood of which the sensitivity of LAI and biomass will be calculatedin the ADAM conditions

parameter	definition	value
dlaimaxbrut	maximum rate of gross leaf surface area production	0.00044
stlevamf	cumulated development units between the LEV and AMF stages	208.298
stamflax	cumulated development units between AMF and LAX stages	181.688
jvc	number of days of vernalisation, expresses the need of cold necessary to lift	35
durvieF	lifespan of a cm of adult leaf	160
adens	parameter to compensate between the number of stems and the density of plants	-0.6
efcroijuv	maximum growth efficiency during juvenile phase (LEV-AMF)	2.2
efcroiveg	maximum growth efficiency during vegetative phase (AMF-DRP)	2.2
efcroirepro	maximum growth effiicency during grain filling phase (DRP-MAT)	4.25
vmax2	maximum rate of nitrate absorption by absorption system 2 (low affinity) in roots	0.05

[a] all the STICS parameters are described in the user guide http://www.avignon.inra.fr/ agro-clim_stics_eng/notices_d_utilisation

[2] The ADAM (Data Assimilation through Agro-Modelling) project and database can be found at http://kalideos.cnes.fr/spip.php?article68

4.2 Sensitivity results of LAI and biomass

Sensitivity analysis of the variable LAI led to the following conclusions (Fig. 2): the most influential parameters on the response function integrating the LAI from those we have considered here are *adens* (47%), *dlaimaxbrut* (21%), *stlevamf* (17%), *jvc* (10%), and finally *stamflax* (2%). *adens* represents the ability of a plant to withstand increasing densities, and since it depends on the species and varieties, its influence may be particularly strong for this type of wheat and less for other crops. For the response function including biomass, we observe that the hierarchy is modified by the strong influence of the efficiency *efcroiveg* (maximum growth efficiency during vegetative phase) which is similar to that of *adens* (27%). This means that we can ignore the estimate of *efcroiveg* if we only want to assimilate LAI data, but absolutely not if we need to simulate biomass. *stlevmaf* and *dlaimaxbrut* are also equivalent (14 and 12%). Finally, there is a relatively low sensitivity (5% and 3%) of biomass integrated over the cycle to the other two parameters of efficiency *efcroirepro* and *efcroijuv*, meaning that the biomass is not so dependant on the juvenile and the grain filling phases but essentially on the vegetative phase. The fact that only the integral over the entire cycle was studied involves a very small influence of the parameters *efcroirepro* and *efcroijuv*, and a most important one of *efcroiveg*. These efficiencies, which are related to phenology are characteristic of certain phenological stages, and it can be assumed that an analysis of the integral of LAI between two consecutive stages only would modify the hierarchy of influent parameters [14].

LAI is actually dependant on 4 parameters and biomasse on 5 on the 10 tested, which will help the user to concentrate on these ones and to estimate them better, allowing to let more uncertainty on the other ones.

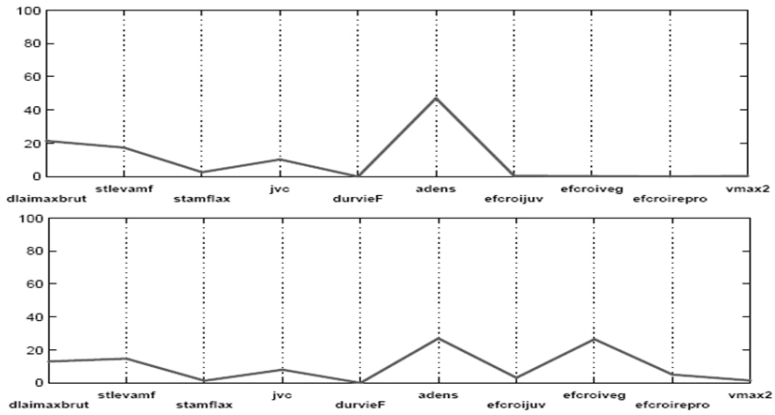

Fig. 2 Relative sensitivity of parameters in % in STICS of the ouput variable Leaf Area Index (LAI, above) and biomass (below) given by the adjoint model run.

5 Conclusion and outlook

This case study illustrates the potential interest of Automatic Differentiation for sensitivity analysis methods for agronomic models. It can as well be used for assimilation of remote sensing data into crop models, for precision agriculture [5], in radiative transfer model [9], by using the adjoint model as a way to minimize the discrepancy cost function. This work shows the feasability of applying and developing variationnal methods in the agronomic field, in the same way it is widely applied in oceanography or meteorology.

For the agronomic community, the adjoint model of STICS is a very interesting tool to perform sensitivity analysis since it requires the calculation only once for each agro-pedo-climatic situation. The most difficult work is the differentiation of the model, which must be done only once, and with the help of AD tools that keep improving. However, the local sensitivity analysis is valid only in a small neighborhood and it is quite possible that the hierarchy would be modified under different conditions. These results are therefore only the first step. Following work could concentrate on:

1. performance of a ”multi-local” sensitivity analysis, keeping the crop management and climate of the base ADAM, in order to generalize the hierarchy of all possible values of the parameters in the ADAM conditions. To do this, the adjoint model has to be run on the set of intervals defining the parameters using a sufficiently representative sample of possible values.
2. application of this analysis to other conditions (climate, soil...) to check that the hierarchy is preserved in general. Extending to other varieties is also important. The generalization of these first results, however, seems unlikely since the change of climate and soil conditions should change the hierarchy of limiting factors (stress for the plant) and thus the influence of certain parameters.
3. study of the sensitivity to several phenological stages of the cycle to study the effect of variables temporally valid (especially efficiency) on the general hierarchy.

The unlimited (within the limits of computational cost) of variable inputs and outputs against which we can calculate the adjoint model gives it a completeness. In fact, the sensitivity analysis will anticipate the lack of determinism of STICS to represent certain processes and guide users’attention on some of STICS modules, parameters or variables according to their objectives. The agronomic field has the special problem to consider the variables of interest (total biomass, yield, balance...) that are not observable by remote sensing. They can not thus be assimilated into the model. The sensitivity analysis will quantify the sensitivity of these variables to those we assimilate (LAI, fAPAR...).

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