Using Automatic Differentiation to study the sensitivity of a crop model

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

Irstea (Environment and Agriculture)
INRIA (Computer Science and Control)
INRA (Agronomy)

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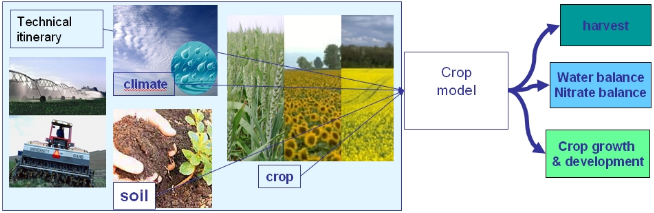
The application domain: the agronomic crop model STICS

STICS simulates the behaviour of the soil-crop system over one or successive crop cycles.



Objectives

to simulate consequences on crop production and environment
of variations in: climate, soil, and crop management

Simulated object (Control Parameters)

a cultural situation = a soil-crop system + a technical itinerary

Simulated processes (Outputs)

- ⇝ growth and development of the crop
- ⇝ water and nitrogen balance of the soil-crop system

Key output variables of STICS

LAI: Leaf Area Index

Total one-sided area of leaf tissue per area of ground surface.

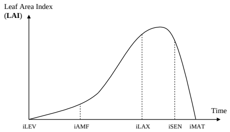
Leaves are the main interface with the atmosphere for the transfer of mass and energy $\Rightarrow$ the LAI indirectly describes:

- potential of photosynthesis available for primary production
- plant respiration, evapotranspiration
- biosphere $\leftrightarrow$ atmosphere carbon flux.
- severely affected areas (fires, parasites. . .)

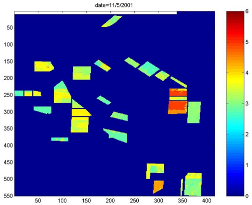
LAI closely related to:

Biomass

Total mass of living matter per area of land.



LAI of wheat over a year



Observed LAI (from inversion of radiative transfer model)

Plan

Sensitivity analysis: what it is and what for?

Sensitivity analysis is an initial goal
$\rightsquigarrow$ further goals include ($\approx$200) parameter estimation

Sensitivity analysis studies the impact of perturbing the control (input) parameters on the model output. It helps to:

- prioritize the model parameters
- identify critical regions in the space of the inputs (including interactions)
- support decision for research and future experiments.
  $\rightsquigarrow$ which parameters deserve accurate measurements?
- gauge model adequacy and physical relevance
- simplify models (metamodeling)
- find technical errors in the model

Sensitivity analysis: mathematical framework

- A model:

$$F(X, K) = 0$$

X = state variables (LAI, biomass ...)
K = control variables (parameters, forcing variables ...)
Here, the *model* is exactly the *STICS computer program* $K \mapsto X$.

- A response function $G(X)$, e.g.
$G_{LAI} = \sum_{i=1}^{T} LAI(t_i)$ or $G_{biomass} = \sum_{i=1}^{T} biomass(t_i)$

The problem is to evaluate the sensitivity of G with respect to K or in other words the gradient of G with respect to K.

With an adjoint model, only 2 steps:

1. run the direct model once for the given K
2. solve the adjoint model

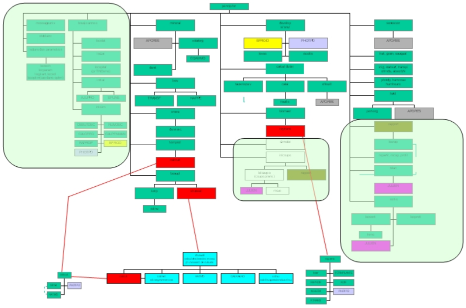
$$\nabla G = \frac{dG}{dK}^t = \left(\frac{dG}{dX}.\frac{dX}{dK}\right)^t = \boxed{\left(\frac{dX}{dK}\right)^t}.\boxed{\left(\frac{dG}{dX}\right)^t}$$

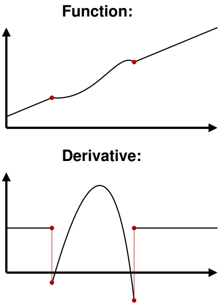
Sensitivity analysis: adjoint model or other approaches?

Adjoint method is the only way to calculate formally the gradient of the response function at a cost that does not depend on the size of K
$\Rightarrow$ appropriate when number of entries $K \gg$ size of response function

other approach	**advantages**	**disadvantages**
tangent-linear	no need to calculate the adjoint	cost proportional to the size of K
finite difference	easy calculations	approximation of the gradient + extensive direct model computations
stochastic sampling techniques	global sensitivity	cost grows rapidly with the dimension of K

Practical problems with models like STICS





Piecewise differentiable function
⇒ only left- and right-derivatives (or sub-gradients)

⇝ Derivative-free methods (divided differences, stochastic,. . .) behave better in these cases, but at a cost.
⇝ In practice, problem is overlooked: local sensitivity valid in a neighborhood of K.

Selected input parameters for sensitivity analysis

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	days of vernalisation (cold days needed to lift)	35
durvieF	lifespan of a cm of adult leaf	160
adens	compensation between number of stems and plants density	-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 the roots	0.05

All these parameters would deserve a good parameter estimation...

Plan

TAPENADE

We build the adjoint of STICS with TAPENADE.

TAPENADE (2.0 at the time, now 3.6):

- Automatic Differentiation by source-to-source transformation
- Flow- and Context-sensitive global data-flow analysis
- Association by name
- Adjoint with Store-All strategy
- Checkpointing on calls by default

A few recommended programming practices

STICS is FORTRAN 77 $\Rightarrow$ In theory, TAPENADE can build its adjoint

- $\rightsquigarrow$ but improvements required on old TAPENADE ($<$ 2005),
- $\rightsquigarrow$ plus some adaption of STICS

Adaption of STICS source:

- Active vars should be separate from others: no big work array !
- Active independents and dependents must be clearly identified $\Rightarrow$ keep them **separate** from the other variables.
- Use a coherent precision level: `DOUBLE PRECISION`
- Solve portability problems unveiled by AD: no uninitialized **remanent globals** !

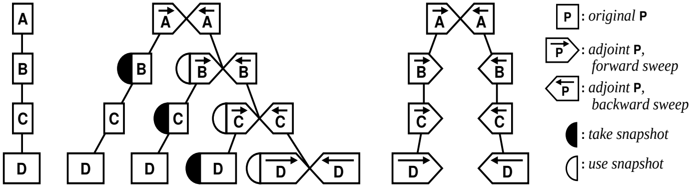
Issues due to AD in general

- *the program itself is the equation* (no ODE/PDE)
  $\Rightarrow$ conditional jumps with no underlying continuity/differentiability.
- Uncontrolled code evolution
  $\Rightarrow$ fast increase of new subcases and subdivisions.

Several subroutines needed manual improvement to Restore differentiability
$\Rightarrow$ a cleaner STICS ?

Issues due to TAPENADE

- Remarkably large number of branches: thresholds, conditions, loops ...that must be stored for control-flow reversal.
  ⇒ define PUSHCONTROL(), cheaper than storing a full INTEGER
- Time stepping: split main time loop (400 steps) into nested 20-steps loops. Make them subroutines to force checkpointing
  ⇒ now with TAPENADE 3.6, use $AD BINOMIAL-CKP
- Fine-tune checkpointing of nested calls:



⇒ $AD NOCHECKPOINT

Co-evolution of STICS and TAPENADE
⇒ a more portable STICS & a more efficient adjoint code

Validation of the adjoint model

Divided Differences:	0.42248278309969720000
Tangent AD:	0.42248278406221984000
Adjoint AD:	0.42248278406222007000

- Performance with TAPENADE 2.0 (2005):

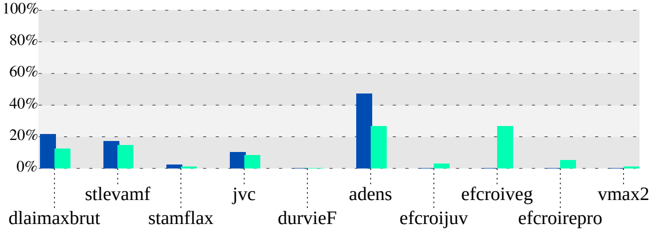
  Orig: 0.21 s   Tgt: 0.39 s   Adj: 30.96 s   Traffic: 13.8 Gb
  Peak: 240 Mb

- After checkpointing fine tuning (`C$AD NOCHECKPOINT`)

  Orig: 0.22 s   Tgt: 0.52 s   Adj: 0.86 s   Traffic: 0.2 Gb
  Peak: 162 Mb

Plan

Sensitivity results of LAI and biomass



Hierarchy of influent parameters:

- LAI: *adens* is the most influential parameter (47%). It represents the ability of a plant to withstand increasing densities, depends on the species and varieties ⇒ strong influence for this type of wheat and less for other crops.
- Biomass: hierarchy modified by the strong influence of the efficiency *efcroiveg* (maximum growth efficiency during vegetative phase) ⇒ we can ignore the estimate of *efcroiveg* if we only work on LAI, but absolutely not to simulate biomass.
- relatively low sensitivity (5% and 3%) of biomass integrated over the life cycle to the other 2 parameters of efficiency *efcroirepro* and *efcroijuv* ⇒ the biomass is not so dependant on the juvenile and the grain filling phases but essentially on the vegetative phase.
- LAI is actually dependant on 4 params and biomass on 5 ⇒ the user should concentrate on these and estimate them better. Uncertainty on the other parameters is of smaller importance.

Conclusion

- For the agronomic community, the adjoint model of STICS is an efficient way to perform sensitivity analysis since it requires the calculation only once for each agro-pedo-climatic situation.
- AD is a choice approach for sensitivity analysis of agronomic models, where the code is the model.
- Sensitivity analysis focuses user's attention on some parameters and modules, according to the user's objectives.
- ! This local sensitivity analysis is local, valid only in a small neighborhood and the hierarchy of sensitivities may vary under different conditions (but in practice: quite stable hierarchy).
- Sensitivity analysis is a preliminary to parameter estimation, data assimilation: many of these agronomic parameters (yield, balance,...) are not directly observable
- This shows that variational methods are applicable in agronomy but it takes a truly pluridisciplinary work!