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Jordi Ferrer Saval
UMR ECOSYS, INRA, UMR MIA-Paris, AgroParisTech, Université Paris-Saclay, jordi.ferrersavall@agroparistech.fr

Pierre Barbillon
UMR MIA-Paris, AgroParisTech, INRA, Université Paris-Saclay

Cyril Benhamou
UMR ECOSYS, INRA, AgroParisTech, Université Paris-Saclay

Patrick Durand
UMR SAS, INRA, Agrocampus Ouest

Marie-Luce Taupin
UMR MaIAGE, INRA, Université Paris-Saclay

See next page for additional authors

Presenter/Author Information

Jordi Ferrer Saval, Pierre Barbillon, Cyril Benhamou, Patrick Durand, Marie-Luce Taupin, Hervé Monod, and Jean-Louis Drouet

International Environmental Modelling and Software Society (iEMSs)
8th International Congress on Environmental Modelling and Software
Toulouse, France, Sabine Sauvage, José-Miguel Sánchez-Pérez, Andrea Rizzoli (Eds.)
http://www.iemss.org/society/index.php/iemss-2016-proceedings

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Jordi Ferrer Savall[ab], Pierre Barbillon[b], Cyril Benhamou[a], Patrick Durand[c], Marie-Luce Taupin[d], Hervé Monod[d] and Jean-Louis Drouet[a]

a: UMR ECOSYS, INRA, AgroParisTech, Université Paris-Saclay, 78850, Thiverval-Grignon, France
b: UMR MIA-Paris, AgroParisTech, INRA, Université Paris-Saclay, 75005, Paris, France.
c : UMR SAS, INRA, Agrocampus Ouest. 84215, Rennes, France
d : UMR MaIAGE, INRA, Université Paris-Saclay, 78350 Jouy-en-Josas, France
jordi.ferrersavall@agroparistech.fr

Abstract: Modelling complex systems such as agroecosystems often requires the quantification of a large number of input factors. Sensitivity analyses are useful to fix the appropriate spatial and temporal resolution of models and to reduce the number of input factors to be measured or estimated accurately. Comprehensive spatial and dynamic sensitivity analyses were applied to the Nitroscape model, a deterministic spatially distributed model describing nitrogen transfers and transformations in a rural landscape. Simulations were led on a virtual landscape that represented five years of farm management in an intensive rural area of 3 km². Cluster analyses were applied to summarize the results of the sensitivity analysis on the ensemble of model outcomes. The 29 studied output variables were split into five different clusters that grouped outcomes with similar response to input factors. Among the 11 studied factors, model outcomes were mainly sensitive to inputs characterizing the lateral transmissivity of soil. The horizontal resolution of the model was a significant factor driving ammonium and nitrate mineralisation, and uptake by plants. The vertical resolution of the model had the highest impact on the cumulate emissions of nitrous oxides. The interactions between the amount of nitrogen used in fertilization and the lateral transmissivity of soil was the most important factorial effect driving the amount of nitrogen in the catchment discharge.

***Keywords**: Se*nsitivity analysis, Cluster Analysis, N cascade, Spatially distributed model, Landscape Scale

1 INTRODUCTION

A main agro-environmental and socio-economic challenge of sustainable agriculture is to maintain agricultural production while reducing the use of nitrogen inputs. The generalized use of artificial nitrogen fertilizers feeds a cascade of processes that releases nitrogen surplus to the local environment and pollutes the air, soils and waterways. Nitrogen losses have a global negative impact on ecosystems, economy and human health causing eutrophication, biodiversity loss, soil acidification and degradation of drinking water sources (Galloway et al., 2003).

A better understanding of the nitrogen cascade in agroecosystems is required in order to find novel ways to reduce losses at each step of the cascade. To this end, mathematical models are developed, evaluated and applied to quantitatively describe nitrogen transfers and transformations at various spatio-temporal scales. Biophysical models are often complex, describing a broad array of phenomena (physical processes, bio-transformations and farm practices), and using a large number of inputs (parameters, initial conditions and continuously-fed data). Determining the resolution and accuracy at which model inputs should be measured or estimated is a matter of great practical importance. Hence, it is necessary to evaluate the influence of model inputs, and more specifically the impact of spatial and temporal resolution, on model outcomes (Bishop et al., 2006).

This work presents a global analysis of sensitivity of the Nitroscape model which describes the cascade of reactive forms of nitrogen (N_r) at the landscape scale. The purpose of this paper is to put forward the methods and preliminary results of a comprehensive spatial and dynamic evaluation of the impact of a set of input parameters on a set of model outcomes. A central concern of the presented work is to provide tools for integrating the results of several multivariate sensitivity analyses on multiple model outcomes.

2 MATERIALS AND METHODS

2.1 The Nitroscape model

Nitroscape is a deterministic, spatially distributed and dynamic model describing N_r transfers transformations in a rural landscape (Duretz et al. 2011). It couples four modules characterizing farm management, biotransformations and transfers by the atmospheric and hydrological pathways. It simulates N_r flows and losses within and between several landscape compartments: the atmosphere, the hydro-pedosphere (groundwater, water table and streams) and the terrestrial agroecosystems (livestock buildings, croplands, grasslands and semi-natural areas).

Nitroscape was applied to a simplified virtual landscape of 300 ha corresponding to an intensive rural area with a succession of maize and wheat crops (125 ha each), pig farming (2 separate buildings, 1 ha each) and unmanaged ecosystems (four plots comprising 48 ha). Topography was characterized by a linear slope with a gradient of 50 m between the highest and the lowest parts of the landscape. Meteorology was characterized by humid climatic conditions and little temperature contrasts. Atmospheric dispersion was not taken into account in the current simulations. Further specifications on the model and the test landscape can be found in Duretz et al. (2011).

Simulations were carried out on daily time steps over a five-year period, starting from January 1st. Simulation outcomes were kept for the analysis of sensitivity after an initialisation period of two years. Daily outcomes were sampled from the catchment outflow and monthly outcomes were sampled throughout the landscape. Spatial outcomes described the local state of the model compartments and local fluxes between compartments with a resolving power set by the model horizontal resolution.

2.2 Experimental design

In order to evaluate the impact of model inputs on model outcomes, 11 parameters were selected, characterizing the spatial resolution of the model (A, B), the physical features of the virtual landscape (C - I) and the agronomic management (J, K). The impact of model inputs was evaluated on 29 model outcomes: 5 variables describing the outflow (*e.g.:* daily nitrogen concentration and amount), 9 spatially-distributed variables describing inter-compartment fluxes (*e.g.*: evapotranspiration, amount of mineralized amonium or nitrate) and 15 spatially-distributed variables describing the local state of the system (*e.g.* amonium or nitrate content in groundwater or in soil).

A complete fractional factorial design (FFD) of size 243 for 11 factors and 3 levels per factor was generated using the R package *Planor* (Kobilinsky et al., 2012). The resulting FFD was a saturated design of resolution 5: with 243 runs, main effects and two-factor interactions could determined for any output variable, with unconfounded factorial effects and zero residual degree of freedom.

2.3 Aggregation of model outcomes

Spatially-distributed outcomes formed large sets that were difficult to handle with conventional statistical tools: each outcome was described by a matrix of size 243 rows x $7 \cdot 10^5$ columns, with each row representing a unit of the FFD and each column a measure on a pixel (under the highest resolution, the virtual landscape comprised 19600 pixels, with 36 monthly samples per pixel).

For this reason, these outcomes were spatially or temporally aggregated to obtain different types of data sets: time-series describing spatially-aggregated outcomes were used to carry out a dynamic sensitivity analysis (Section 3.1), while maps of temporally aggregated outcomes were used in a spatial sensitivity analysis (Section 3.2). All the outcomes were also spatially and temporally aggregated in order to carry out a synthesis of the results of the sensitivity analyses applied on the ensemble of model outcomes (Section 3.3).

2.4 Principal Component Analysis

The principal component analysis (PCA) is a procedure to transform any set of possibly correlated variables into a set of values of linearly uncorrelated variables called principal components (PC). Geometrically speaking, the PCA transforms data to a new orthogonal coordinate system such that the greatest variance by projection of the data comes to lie on the first axes of the new coordinate system (first PCs). In the current paper, PCA was used with two different purposes.

Firstly, outcome data sets show strong correlations arising from model structure. PCA was applied on each aggregate outcome to reduce data redundancy and to identify signs of the model structure, such as seasonality in time series (Section 3.1) or land-use attribution in maps (Section 3.2).

Secondly, PCA was applied on the ensemble of sensitivity analysis results of the ensemble of temporally and spatially aggregated outcomes, to better visualize the outcomes that had a similar response to input factors and to evaluate the relationship between the overall effects of different factors. The R package *FactoMineR* was used to carry out this analysis (Section 3.3).

2.5 Analysis of sensitivity

The influence of factors on model outcomes was explored through a standard analysis of variance (ANOVA) on each output variable (expressed as an aggregated data set or in terms of its principal components) considering up to second-order interactions. The R package *Multisensi* (Lamboni et al., 2011) was used.

For each outcome, the fraction of variance among simulations explained by the variation of each factor was quantified by the sensitivity indexes for the main effects (mSI) and for pairwise interactions. For each factor, the total sensitivity index (tSI) was computed as the sum of its main effect and the ensemble of its pairwise interactions (iSI). Given that the proposed FFD was saturated, there was no residual variance: for each outcome, the sum of pairwise interactions (i_{TOT}) and main effects of all factors added up to 100% of the total variance.

2.6 Cluster analysis

Clustering is a procedure to group a set of objects in such a way that objects in the same group are more similar to each other (according to some defined metric) than to those in other groups. In the current paper, clustering methods were used with two different purposes.

Firstly, for each outcome, the 243 time-series obtained for the different runs of the FFD were split into three clusters that grouped curves with similar features (*e.g.:* slope, range of variation, etc.). These clusters were compared to the classifications associated with the levels of each factor. Chi-square tests for independence were applied to evaluate whether the time-series clusters were correlated with the levels of any factor, *i.e.*: to test if any level of any factor could be associated with time-series having a particular feature (Section 3.1).

Secondly, cluster analysis was applied on the ensemble of sensitivity analysis results of the ensemble of temporally and spatially aggregated outcomes, to identify groups of outcomes with similar profiles of sensitivity indices. The R package *FactoMineR* was used to carry out this analysis (Section 3.3).

3 RESULTS AND DISCUSSION

Two samples of the detailed analysis of sensitivity applied on every Nitroscape outcome are presented next. Section 3.1 presents the dynamic sensitivity analysis of a spatially-aggregated inter-compartment flux: the amount of nitrous oxides emitted by the landscape every month. Section 3.2 presents the spatial sensitivity analysis of a temporally aggregated local state variable: the average nitrate concentration in the soil mineral pool at 60 cm depth. The results of the analysis of sensitivity of the ensemble of Nitroscape outcomes, spatially and temporally aggregated, are summarized in Section 3.3.

3.1 Dynamic sensitivity analysis

Figure 1 outlines the detailed results for the dynamic analysis of sensitivity of the variable "Cumulated NOx emissions". The analysis below was applied on every outflow variable and spatially aggregated outcome. Extracting conclusions from the ensemble of results of the dynamic sensitivity analyses was out of the scope of this work. An equivalent synthesis for all outcomes is presented in Section 3.3.

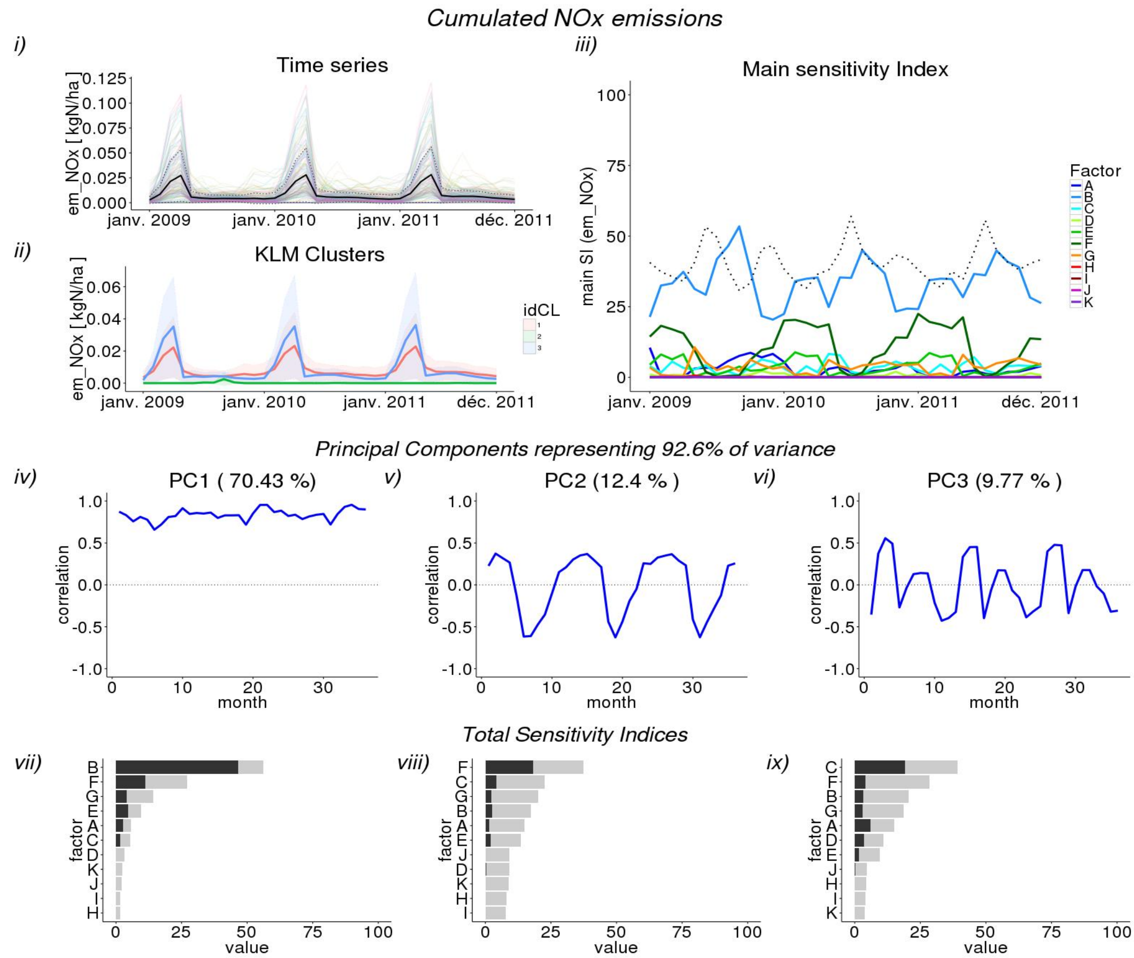

Figure 1: Dynamic analysis of sensitivity for NOx emissions. i) Time series of each simulated run (colored lines), average (bold black line) and inter quantile range (dashed black line); ii) Time-series of 3 clusters grouping most-similar curves; iCL: cluster label. iii) Dynamic main sensitivity indexes of each factor (colored lines) and of the sum of interactions (dashed black line). Global sensitivity analysis: (iv-vi) decomposition of the first three principal components (PC); (vii-ix) total sensitivity indexes of each factor on each PC, split into main effect (black) and interaction (grey) terms.

Figure 1 can be interpreted as follows:

- time series showed peaks of NOx emissions during spring (fertilisation period);
- clusters grouped time-series based on their mean-over-time, range of peaks and dynamic variance. This classification could not be considered independent from the splitting by levels of factors A, C, E, F and G;
- NOx emissions were mostly sensitive to factor B -the vertical resolution- (mSI_B = (45 ± 6)%) ; they were equally sensitive to the sum of pairwise interactions (i_{TOT} = (41 ± 6)%);
- PC1 represented the mean-over-time of time-series. It was mainly sensitive to the main effects of factors B and F;
- PC2 showed 1-year periodicity and a strong correlation with the peaks of time-series and a strong correlation with the peaks of time-series. It reflected the main effect of factor F and the interactions C:G, A:B and B:F
- PC3 showed 6-month seasonality with peaks on the extremes of PC2. It reflected the main effect of factor C and the interactions F:G, B:C and C:F.

3.3 Spatial sensitivity analysis

Figure 2 outlines the detailed results for the spatial analysis of sensitivity of the variable "Average amount of nitrate in the soil mineral pool at 60cm".

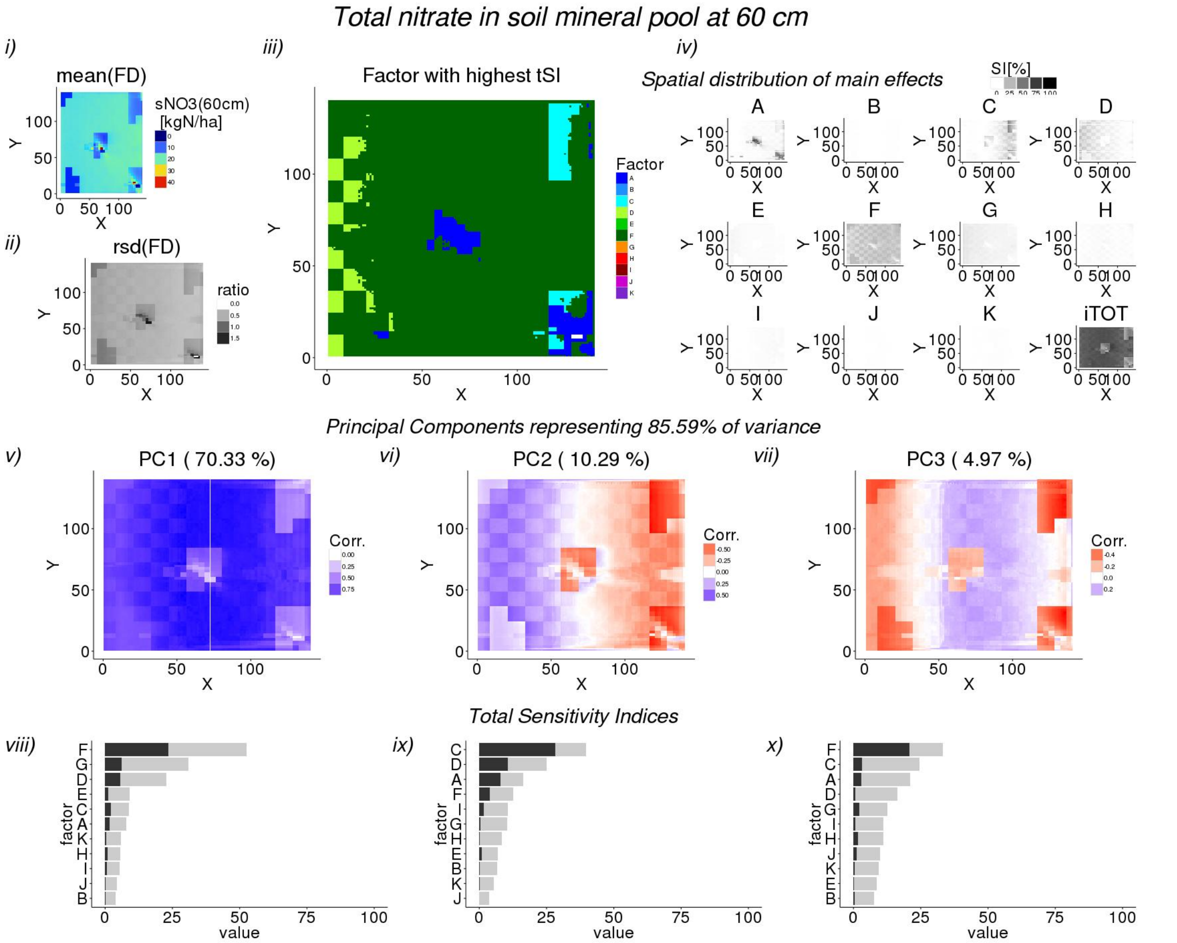

Figure 2: Spatial sensitivity analysis of nitrate concentration at a 60cm depth. i) map of averages over time and over the factorial design. ii) rsd: coefficient of variation between runs of the factorial design; iii) map of the factors with the highest total sensitivity index (tSI) at each pixel; iv) maps of the main effects of each factor and of the sum of interactions (i_{TOT}); global sensitivity analysis: (v-vii) decomposition of the first three principal components; viii-x) total sensitivity indexes of each factor on each PC, split into main effect (black) and interaction (grey) terms.

Figure 2 can be interpreted as follows:

- average nitrate concentration was smaller for unmanaged plots than for crops and it presented local maxima around farm buildings;
- the variance of the FFD was greater in unmanaged parcels and around farm buildings, indicating that these areas were more sensible to model inputs;
- the factors with highest impact were spatially distributed. Locally most important factors were: size of the horizontal spatial mesh (A) around farm buildings, lateral transmissivity of soil (C) in unmanaged parcels downslope, exponential decrease in soil transmissivity with depth (D) in some croplands upslope, and the porosity of soil (F) elsewhere;
- the main sensitivity indexes were spatially distributed accordingly, and interactions had significant impact everywhere;
- PC1 described the spatial mean of FFD variance and it was mostly sensitive to the main effect of factor F as well as most of the interaction terms;
- PC2 was positively correlated with unmanaged plots downslope and negatively correlated with croplands upslope; it was sensitive mainly to the main effects of factors C and D;
- PC3 was positively correlated with unmanaged plot and with croplands upslope; it was sensitive to the main effects of factor F and its interactions.

3.3 Global sensitivity analysis for multiple outcomes

A cluster analysis was applied to the ensemble of spatially and temporally aggregated outcomes to group outcomes with similar response to the ensemble of factors (Kaufman, 2009) .

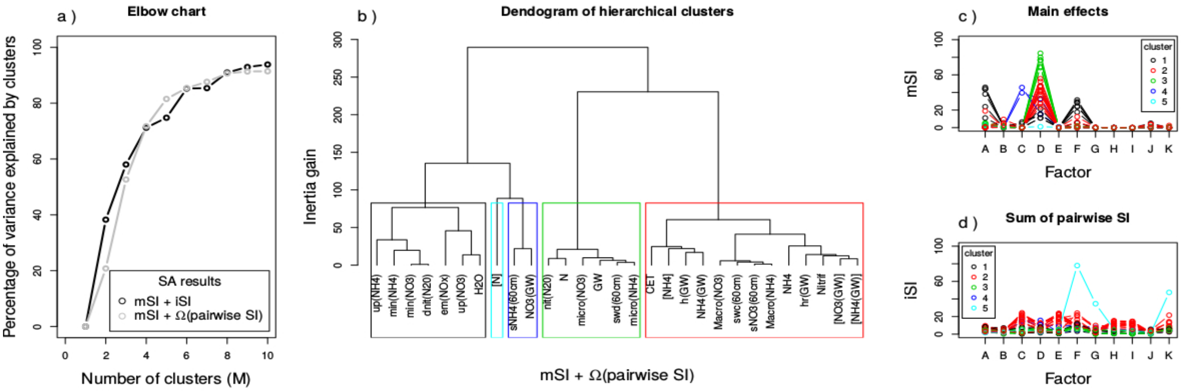

Figure 3: Cluster analysis of the NitroScape outcomes based on their global sensitivity index profiles: a) Percentage of variance explained by clusters as a function of the number M of clusters; black line: SA results are expressed in terms of main effects (mSI) and sum of pairwise interactions (iSI) of each factor; grey line: SA results are expressed in terms of main effects of each factor and the ensemble of pairwise interaction terms Ω(pairwise SI); b) hierarchical clustering of outcomes: outcomes are linked together if they have similar profiles of sensitivity indices; Inertia gain: variance explained when outcomes are linked together. Colour boxes indicate the clusters obtained for M = 5; c) main effects of each factor on each outcome; d) sum of pairwise interactions of each factor on each outcome. Colours of each line are set according to the colours of clusters.

The number of clusters (M=5) was selected with the elbow method (with 81.3% of variance explained). It also corresponds to the number of clusters that provides equal classifications of outcomes with different clustering methods.

In order to better visualize the clusters of similar outcomes and the relations between the effects of each factor, a PCA was applied to transform the space of sensitivity indexes. The projections of outcomes and sensitivity indexes on the axes of the transformed space are shown in Figure 4.

The projection PC1-PC2 shows that 70% of the variance of the sensitivity indexes was explained by this projection (Fig. 4a and 4d). It allowed discriminating clusters 1, 2 and 3. Cluster splitting was driven by the main effects of factors D, F and A. In this projection, the main effects of each factor were independent from each other (indicated by the orthogonal projections of their indexes).

The projection PC1-PC3 explained 60% of the variance (Fig. 4b and 4e). It allowed discriminating clusters 1 and 3 along the axis $\overline{D(A,F)}$ and clusters 4 and 5 along the axis $\bar{C}$. Cluster splitting was driven by the main effects of factors A, C, D and F (Fig. 4e). The effect of factor C was independent from the main effect of other factors and negatively correlated with the effects of pairwise interactions (indicated by anti-parallel projections of their indexes). Main effects of factors A and F were negatively correlated with the main effect of factor D (where the later had a high impact on the outcomes the former did not, and vice versa).

The projection PC2-PC3 explained 30% of the variance (Fig. 4c and 4f).. It allowed discriminating clusters 4 and 5. Cluster splitting was driven by the main effects of factors A, C, D and F, and by the pairwise interactions A:F, C:E, F:G and F:K (Fig. 4f). Factor C was independent from the other factors, the main effects of factors A, D and F were negatively correlated with pairwise interactions.

Table 1 summarizes the results of the cluster analysis and the PCA applied on the ensemble of spatially and temporally aggregated outcomes, characterized by their sensitivity indexes. Some closing remarks regarding this synthetic analysis are discussed next.

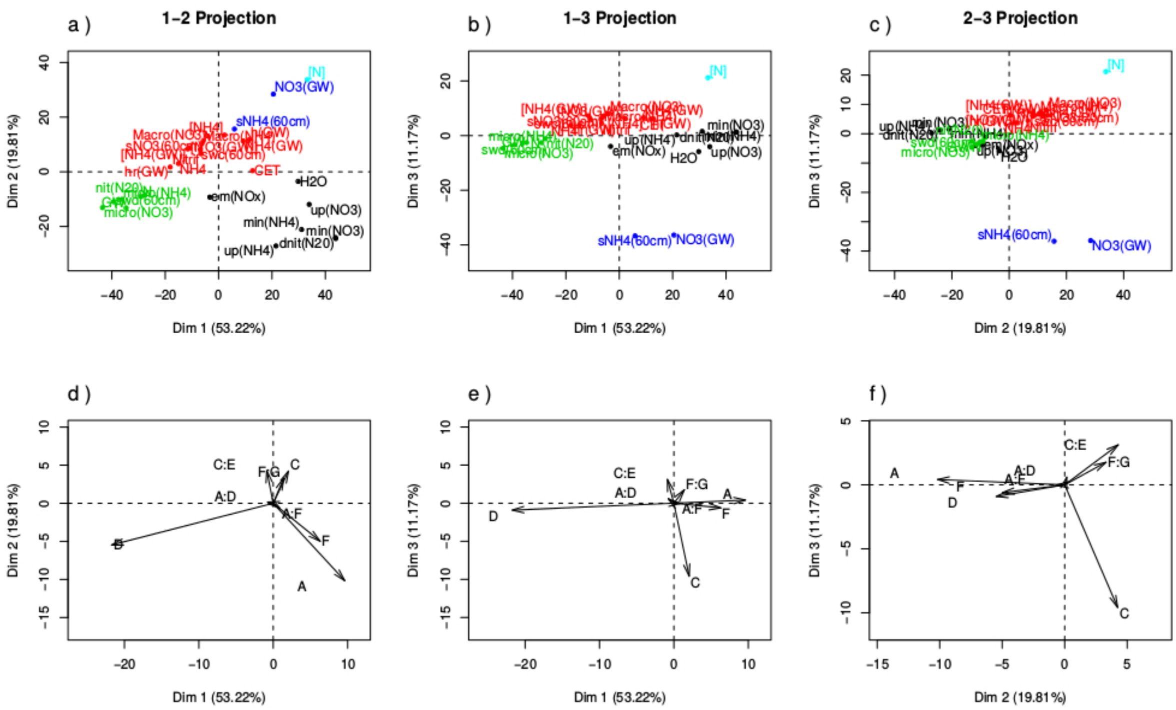

Figure 4: Principal Component Analysis and clustering of the results of the global sensitivity analysis of NitroScape. a - c) projections of the clusters of outcomes onto the plane defined by two principal components; d - f) projections of sensitivity indexes of input factors onto the plane defined by the principal components.

Cluster	N (k)	Outcomes	Characteristics
k = 1	6	*H_2O, up(NO_3), up(NH_4), min(NO_3), min(NH_4), dnit($N_2$0)*	Mostly affected by the porosity of soil (factor F), the horizontal spatial resolution of the model (factor A) and the decrease in soil transmissivity with depth (factor D). Moderate impact of interaction terms.
k = 2	14	*NH_4, [NH_4], em(NOx), Nitrif, CET, swc(60cm), SNO$_3$(60cm)), h(GW), hr(GW)), [NO$_3$(GW)], NH$_4$(GW), [NH$_4$(GW)], Macro(NH$_4$), Macro(NO$_3$)*	Mostly affected by the decrease in soil transmissivity with depth (factor D) and the porosity of soil (factor F). High impact of all interaction terms.
k = 3	6	*N, nit($N_2$0), swd(60cm), GW, micro(NH$_4$), micro(NO$_3$)*	Mostly affected by the porosity of soil (factor F). Low impact of interaction terms.
k = 4	2	*sNH$_4$(60cm), NO$_3$(GW)*	Mostly affected by the lateral transmissivity of soil (factor C) and the decrease in soil transmissivity with depth (factor D). Moderate impact of interaction terms, mainly associated to factor D.
k = 5	1	*[N]*	Mostly affected by the interaction between the lateral transmissivity of soil (factor F) and the amount of Nitrogen in fertilization (factor K)

Table 1: Summary of the results of the clustering analysis and the principal component analysis applied to the global sensitivity indexes of the ensemble of NitroScape outcomes. N(k): number of outcomes in cluster k.

Clusters grouped variables that were sensitive to the same factors. However, this did not entail that factors affected these variables in the same way. For example, *sNH$_4$(60cm)* and *NO$_3$(GW)* were grouped together in cluster 4 as they both had a high sensitivity to the lateral transmissivity of soil (factor C), but while *sNH$_4$(60cm)* decreased when C increased, *NO$_3$(GW)* increased with C.

The horizontal resolution of the model (A) was the factor that had the highest main effect on the spatially and temporally aggregated outcomes describing nitrous oxide consumed by denitrification and ammonium / nitrate mineralisation and uptake by plants. The vertical resolution (B) was the factor that had the third highest total impact on the spatially and temporally aggregated cumulate NOx emissions. The soil physical parameter to which Nitroscape outcomes were the most sensitive was porosity (F), although lateral water transmissivity (C) and its decrease with depth (D) played significant roles. The total amount of nitrogen fertilizer (K) was the only parameter describing agronomic management that had a significant impact on the model results. Its impact was mediated through the interaction with the lateral transmissivity of soil (C:K): the amount of fertilisation was higher under soils with high transmissivity.

4 CONCLUSIONS AND FUTURE WORK

We developed a procedure to perform and synthesize a comprehensive spatial and dynamic analysis of sensitivity of a complex model with several input factors and outcome variables. Some general conclusions regarding the applicability of this analysis are presented below. The methods here presented offer many opportunities for future development. Some of them are listed next.

The detailed spatial and dynamic analyses of sensitivity of model outcomes provided a thorough characterisation of each output variable. The synthesis of results for spatially and temporally aggregated variables permitted classifying outcomes based on their responses to input parameters. Conversely, it allowed classifying parameters based on their influence on each type of outcome and ruling out parameters that have no influence on the outcomes, within the range of explored values.

In order to perform the detailed global analyses of sensitivity for each outcome, variables were aggregated either spatially or temporally. Other types of data aggregation could be applied: for instance, data could be aggregated by land use, selecting those pixels that hold a particular crop at a particular time. This could be used to compare different types of agronomic management.

The detailed spatial and dynamic analyses of sensitivity of each model outcome were here presented for two sample outcomes only. Any other outcome could be thoroughly characterized this way.

Due to space limitations, the cluster analysis and principal component analysis used to summarise the results of the sensitivity analyses on the ensemble of outcomes was here presented only for spatially and temporally aggregated variables. This synthesis could be easily extended to any set of outcomes characterized by any set of sensitivity indexes, in particular, by those resulting from the dynamic or spatial sensitivity analysis.

ACKNOWLEDGMENTS

This work was supported by the French Research Agency (ANR), program "Agro-biosphere sustainability and adaptation of productive ecosystems in response to global climate change - 2012", project ESCAPADE (ANR-12-AGRO-0003).

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Appendix Tables: Description of NitroScape parameters and outcome variables

Factor	Description	Levels	Unit
A	Mesh width (horizontal resolution)	{12.5, 25, 50}	*m*
B	Soil depth (vertical resolution)	{0.02, 0.05, 0.1}	*m*
C	Lateral transmissivity of soil	{2, 8, 15}	*m²/day*
D	Depth of exponential decrease in transmissivity	{0.001, 0.01, 0.1}	*m*
E	Surface layer depth (HS)	{0.2, 0.3, 0.4}	*m*
F	Total porosity of surface layer threshold	{0.12, 0.24, 0.48}	-
G	Ratio of microporosotity to macroporosity	{0.5, 1, 1.2}	-
H	Intermediate layer depth (HI)	{0.6, 0.9, 1.2}	*m*
I	Ratio of microporosotity HI / HS	{1, 0.75, 0.5}	-
J	Type of nitrogen fertilization	{OL, OF, INO}	-
K	Amount of nitrogen in fertilization	X +- 20%	*kg(Nr)/ha*

Table A1: NitroScape input parameters that were varied in the experimental design. *Nr*: anthropogenic reactive forms of nitrogen, *OL:* organic liquid manure, *OF*: organic solid fertilizer, *INO*: inorganic mineral fertilizer. Levels of the amount of *Nr* in fertilization are set within a 20% range around a fixed value (X) that depends on the type of fertilization, the number of applications and the type of crop (average value: 180 kg(N_r) $ha^{-1}year^{-1}$).

Name	Description	Unit	Type
em(NOx)	Nitrogen oxides emissions	kg(N)/ha	flow
Nitrif	Net production of nitrous oxide	g(N)/ha	flow
up(NO_3)	Plant nitrate uptake	kg(N)/ha	flow
up(NH_4)	Plant ammonium uptake	kg(N)/ha	flow
CET	Cumulative total evapotranspiration	mm	flow
min(NH_4)	Mineralized ammonium	kg(N)/ha	flow
min(NO_3)	Mineralized nitrate	kg(N)/ha	flow
dnit($N_2$0)	Nitrous oxide consumed by denitrification	kg(N)/ha	flow
nit($N_2$0)	Nitrous oxide produced by nitrification	kg(N)/ha	flow
swc(60cm)	Soil water content at 60 cm	m	state
swd(60cm)	Soil water volume fraction at 60 cm	m	state
sNO_3(60cm)	Nitrate content in soil mineral pool at 60 cm	kg(N)/ha	state
sNH_4(60cm)	Amonium content in soil mineral pool at 60 cm	kg(N)/ha	state
GW	Total groundwater content	m	state
h(GW)	Groundwater depth	m	state
hr(GW)	Groundwater depth of reference	m	state
[NO_3](GW)	Concentration of nitrate in groundwater	kg(N)/ha	state
NO_3(GW)	Amount of nitrate in groundwater	kg(N)/ha	state
[NH_4](GW)	Concentration of amonium in groundwater	kg(N)/ha	state
NH_4(GW)	Amount of amonium in groundwater	kg(N)/ha	state
Macro(NO_3)	Nitrate adsorbed by macroporosity of alterites	kg(N)/ha	state
Macro(NH_4)	Amonium adsorbed by macroporosity of alterites	kg(N)/ha	state
micro(NO_3)	Nitrate adsorbed by microporosity of alterites	kg(N)/ha	state
micro(NH_4)	Amonium adsorbed by microporosity of alterites	kg(N)/ha	state
H_2O	Catchment discharge	m³	outflow
[N]	Nitrogen concentration in catchment discharge	kg(N)/m³	outflow
[NH4]	Amonium concentration in catchment discharge	kg(N)/m³	outflow
N	Nitrogen content in catchment discharge	kg(N)	outflow
NH4	Amonium content in catchment discharge	kg(N)	outflow

Table A2: NitroScape outcomes. Flow and state variables are dynamic (with monthly samples) and spatially distributed. Outflow variables are dynamic (with daily samples).