Sensitivity analysis of spatio-temporal models describing nitrogen transfers, transformations and losses at the landscape scale

Jordi Ferrer Savall¹, Damien Franqueville¹, Pierre Barbillon∗², Cyril Benhamou¹, Patrick Durand³, Marie-Luce Taupin⁴, Hervé Monod², and Jean-Louis Drouet¹

¹UMR ECOSYS, INRA, AgroParisTech, Université Paris-Saclay, 78850, Grignon, France.
²UMR MIA-Paris, AgroParisTech, INRA, Université Paris-Saclay, 75005, Paris, France.
³UMR SAS, INRA, Agrocampus Ouest. 84215, Rennes, France.
⁴UMR MaIAGE, INRA, Université Paris-Saclay, 78350 Jouy-en-Josas, France.

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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 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 rural landscapes. Simulations were led on a virtual landscape that represented five years of intensive farm management and covering an 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 the inputs characterizing the type of fertilization and the hydrological features of soils. The total amount of nitrogen in the catchment discharge was the type of nitrogen used in fertilization, while nitrogen concentration in catchment discharge was mainly driven by soil porosity and lateral water transmissivity. The vertical resolution of the model had a significant impact on the ammonium surface content and on the nitrate groundwater concentration, while the model horizontal resolution had a significant impact on the

∗Corresponding author: pierre.barbillon@agroparistech.fr
dynamic and spatial distributions of model outcomes, but it did not significantly affect nitrogen variables when they were spatially- and temporally-aggregated. The methodology we applied should prove useful to synthesise sensitivity analyses of models with multiple space-time input and output variables.

**Keywords:** Sensitivity analysis, Cluster analysis, Nitrogen cascade, Spatial 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 cycle 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. Agro-environmental 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). To accurately estimate these input factors, a large amount of data is required and the field measurements that provide these data are time-consuming and costly [Drouet et al., 2011].

Therefore, determining the resolution at which model inputs should be measured or estimated is a matter of great practical importance both for the statistical interpretation of field data, and for the meaningful communication of model predictions. Likewise, since the precision of simulations with respect to space and time may influence the model outcomes, the optimal spatial granularity and temporal accuracy at which simulations should be run has to be determined prior to using any model to assess mitigation options on real systems. Hence, the impact of the spatial and temporal resolution of simulations should be evaluated together with the impact of uncertainty in model inputs, and their effects on model outcomes should be quantitatively compared with each other [Bishop and Lark, 2006].

Up to date, a wide variety of techniques have been developed to perform sensitivity analysis in spatially and dynamic models at different stages [Faivre et al., 2013]. Methods for exploring model inputs may range from the simplest one-factor-at-a-time screening techniques proposed by Morris [1991] to complete factorial designs [Chen and Cheng, 2011]. Sensitivity analyses may also focus only on the variation in model inputs or in their spatial distribution [Marrel et al., 2011]. Variance-based methods of the impact of inputs on outcomes may be dynamic and spatially explicit or expressed in terms of global sensitivity indexes [Moreau
et al., 2013). Finally, outcomes may be considered at a fine scale or aggregated at different scales of description (Ligmann-Zielinska, 2013).

The purpose of this paper is to provide some novel analytical and visualization methods to carry out a comprehensive evaluation of the impact of a set of globally defined input parameters on a set of spatially distributed model outcomes, together with the assessment of the impact of the spatial accuracy of simulations. A central concern of the current work is to put forward some tools that allow integrating the results of several sensitivity analyses carried on multiple model outcomes into a single indicator.

In order to do this, we present a case study of a global sensitivity analysis of a model describing the cascade of reactive forms of nitrogen ($N_r$) at the landscape scale, where we evaluate the impact of the spatial resolution of the model, the physical features of the landscape and the agricultural management procedures, on several spatially-distributed outcomes describing the nitrogen cycle, such as the amount of ammonium and nitrate fixation and assimilation, the atmospheric emissions or the amount of nitrogen released in the catchment discharge.

2 Materials and methods

2.1 The NitroScape model

NitroScape is a deterministic, spatially distributed and dynamic model describing $N_r$ transfers and transformations in rural landscapes (Duretz et al., 2011). It couples four modules characterizing farm management, biotransformations and transfers by the atmospheric and hydrological pathways (Figure 1a). It simulates flows and losses of nitrogen reduced forms ($NH_3$, $NH_4^+$), inorganic oxidized forms ($NO_3^-$ and $N_2O$) and organic forms (manure, vegetation and crop residues) within and between several landscape compartments: the atmosphere, the hydro-pedosphere (soil, water table, groundwater and streams) and the terrestrial agroecosystems (livestock buildings, croplands, grasslands and semi-natural areas).

NitroScape was applied to model the nitrogen cycle in a simplified virtual landscape (Figure 1b) of 300 ha corresponding to an intensive rural area with a succession of maize and wheat crops in a checkerboard distribution (125 ha each crop), pig farming facilities (2 separate buildings, 1 ha each) and unmanaged ecosystems (four plots, scattered along the landscape and comprising 48 ha in total). 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. Meteorological data used for the simulation were measured with a meteorological station located on the Kervidy-Naizin catchment ($48^\circ 01'N, 2^\circ 83'O$) between 2007 and 2011. Atmospheric dispersion was not taken into account in the current simulations. Further specifications on the model and the virtual 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, 2007. Simulation outcomes were kept for the sensitivity analysis after an ini-
Figure 1: Scheme of the NitroScape model (a) Land use and topography in the virtual landscape (b), *: catchment discharge.
tialization 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 Design of numerical experiments

In order to evaluate the impact of model inputs on model outcomes, 11 parameters were selected (Table 1), 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. evapo-transpiration, amount of mineralized ammonium or nitrate) and 15 spatially-distributed variables describing the local state of the system (e.g. ammonium or nitrate content in groundwater or in soil).

| 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 (HS) depth                                | 0.2, 0.3, 0.4  | m      |
| F      | Total porosity of surface layer threshold               | 0.12, 0.24, 0.48|        |
| G      | Ratio of microporosity to macroporosity                 | 0.5, 1, 1.2    |        |
| H      | Intermediate layer (HI) depth                           | 0.6, 0.9, 1.2  | m      |
| I      | Ratio of microporosity 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 1: 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 were set within a 20% 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(Nr)ha⁻¹year⁻¹).

A 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 consisted of a carefully chosen subset of the simulation runs so as to expose the single factor effects and two-factor interactions. A complete saturated design of resolution 5 could be obtained: for every output variable, this design allowed determining the main effects and two-factor interactions with single and pairwise factorial effects unconfounded and with no residual degrees 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 · 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). The R package Multisensi (Lamboni et al., 2009) was used to carry out this analysis.

Secondly, PCA was applied on the ensemble of sensitivity indexes of the ensemble of temporally- and spatially-aggregated outcomes, in order 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 (Lé et al., 2008) was used to carry out this analysis (Section 3.4).

2.5 Sensitivity analysis

The influence of factors on model outcomes was explored through a standard analysis of variance (ANOVA) on each output variable considering up to two-factor interactions. The R package Multisensi (Lamboni et al., 2011) was used to carry out this generalized sensitivity analysis of each simulation outcome, expressed either as spatially explicit dynamic data set or in terms of their principal components.

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).

The FFD being saturated, no residual variance was found: for each outcome, the sum of the main effects of all factors and of the ensemble of pairwise interactions (iTOT) added up to 100% of the total variance explored by the experimental design. Therefore, iTOT was used as a direct measure of the variance that could not be attributed to any single factor.

2.6 Cluster analysis

While PCA is used to give a reduced set of attributes that reflect the most variation of data, clustering is a procedure used to define groups of similar objects, based on their attribute values (Kaufman and Rousseuw, 2009). 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). 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 results of the sensitivity analyses of all temporally- and spatially-aggregated outcomes, in order to synthesize the results obtained for the ensemble of outcomes. The R packages FactoMineR and PVclust (Suzuki and Shimodaira, 2006) were used to carry out this classification (Section 3.4).

The joint application of cluster analysis and PCA provides representations that allow identifying groups of outcomes with similar profiles of sensitivity indexes and better visualizing the relations between the effects of input factors on the ensemble of outcomes. In these representations, orthogonality between the projections of the sensitivity indexes of two factors indicates the independence of the factors: outcomes may be affected by either factor, by both of them or by neither of them. On the other hand, the parallel projection of two factors’ sensitivity indexes indicates that whenever one of the factors has an impact on an outcome, the other factor has an impact too. Finally, the antiparallel projection of two factors’ sensitivity indexes indicates that whenever one of the factors has an impact on an outcome, the other factor does not have an impact, and vice versa.

3 Results and Discussion

Some examples of the detailed sensitivity analysis applied on each NitroScape outcome are presented next. Section 3.1 compares the dynamic sensitivity analysis of two spatially-aggregated variables. Section 3.2 compares the spatial sensitivity analysis of two temporally-aggregated variables. The correspondence between spatial and dynamic sensitivity analyses is briefly discussed in Section 3.3.
The results of the sensitivity analysis of the ensemble of NitroScape outcomes, spatially- and temporally-aggregated, are summarized in Section 3.4. Extracting conclusions from the ensemble of results of the detailed spatial and dynamic sensitivity analyses is out of the scope of this work.

3.1 Dynamic sensitivity analysis

A dynamic sensitivity analysis was applied on every spatially-aggregated outcome as well as on each outflow variable. Figure 2 outlines the detailed results for the dynamic sensitivity analysis of an inter-compartment flux \( i.e. \) the variable 'Cumulated NO\(_x\) emissions' describing the total amount of nitrogen oxides produced by the whole landscape. Figure 3 outlines the detailed results for the variable 'Cumulative NH\(_4\) plant uptake', \( i.e. \) the amount of ammonium absorbed by all plants throughout the landscape.

Some remarks can be extracted from Figures 2 and 3:

i Time series showed peaks of both NO\(_x\) emissions and NH\(_4\) uptake by plants during the fertilization periods at spring;

ii Clusters grouped time-series based on their mean-over-time, range of peaks and dynamic variance. This classification was apparent for NH\(_4\) uptake but could not be appreciated for NO\(_x\) emissions;

iii NO\(_x\) emissions were mostly sensitive to the vertical resolution of the model (factor B: \( mSI_B = (41 \pm 7\)%\)) and to the sum of pairwise interactions (\( i_{TOT} = (28 \pm 6\)%\)); NH\(_4\) uptake was mostly affected by pairwise interactions of multiple factors (\( i_{TOT} = (56 \pm 18\)%\)), but also sensitive to the main effects of the surface porosity (factor F), to the type of nitrogen fertilization (factor J) and to the lateral transmissivity of soil (factor C);

iv PC1 represented the mean-over-time of time-series. For NO\(_x\) emissions, this component was mainly sensitive to the main effects of the vertical resolution (factor B), while for NH\(_4\) uptake the greatest contributions to its variation come from pairwise interactions involving surface porosity and type of fertilization (factors F and J);

v PC2 revealed the factors that mostly affect time series with one-year periodicity (\( e.g. \) the factors that mostly affect time series during spring). For NO\(_x\) emissions, this component mainly reflected the effects of porosity (factor F) and type of fertilization (factor J), as well as their pairwise interactions. For NH\(_4\) uptake, this component was mainly affected by the main effects and pairwise interactions of the lateral transmissivity of soil.

vi PC3 captured effects with smaller seasonality, showing peaks of representation on the zeros of PC2. For NO\(_x\) emissions, it captured the effects of the lateral transmissivity of soil (Factor C). For NH\(_4\) uptake, it mainly captured the ensemble of pairwise interactions.

To sum up, the detailed dynamic sensitivity analysis above allowed assessing how each input factor affected the evolution of each whole-landscape nitrogen outcome.
Figure 2: Dynamic sensitivity analysis for NO\textsubscript{x} emissions. a) Time series of each simulated run (colored lines), average (bold black line) and inter quantile range (dashed black line); b) Time-series of 3 clusters grouping most-similar curves; idCL: cluster label. c) Dynamic main sensitivity indexes of each factor (colored lines) and of the sum of interactions (dashed black line). Global sensitivity analysis: d-f) decomposition of the first three principal components (PC); g-i) total sensitivity indexes of each factor on each PC, split into main effect (black) and interaction (gray) terms.
Figure 3: Dynamic sensitivity analysis for ammonium uptake. a) Time series of each simulated run (colored lines), average (bold black line) and inter quantile range (dashed black line); b) Time-series of 3 clusters grouping most-similar curves; idCL: cluster label. c) Dynamic main sensitivity indexes of each factor (colored lines) and of the sum of interactions (dashed black line). Global sensitivity analysis: d-f) decomposition of the first three principal components (PC); g-i) total sensitivity indexes of each factor on each PC, split into main effect (black) and interaction (gray) terms.
3.2 Spatial sensitivity analysis

Figure 4 outlines the results for the spatial sensitivity analysis of the local state variable 'Average amount of nitrate in the soil mineral pool at a 60 cm depth'. Figure 5 outlines the results for the spatial sensitivity analysis of the local flux variable 'Cumulative NH$_4$ plant uptake', representing the total amount of nitrogen captured at each pixel.

Some remarks can be extracted from Figures 4 and 5:

i. Both the surface nitrate concentration and the ammonium uptake were smaller for unmanaged plots than for crops and presented local maxima around farm buildings;

ii. Conversely, the relative variance was greater in unmanaged parcels and around farm buildings, indicating that these areas were more sensitive to model inputs;

iii. For both variables, the factors with the highest effect were spatially distributed. The size of the horizontal spatial mesh (factor A) is the most important around farm buildings and on the edges of the landscape. Elsewhere, the most important factors varied depending on altitude and land use. Generally, the most important factor for both variables was the porosity of the surface layer (factor F), although the type of fertilization (factor J) was the paramount factor for maize crops located upslope;

iv. The maps of the distribution of main sensitivity indexes for each factor were in accordance with the previous results. For both variables, the role of the ensemble pairwise interactions had the most significant effects throughout the landscape;

v. For both variables, PC1 described the spatial mean of FFD variance. This component was mostly sensitive to the main effect of surface porosity (factor F) and to its pairwise interaction terms;

vi. For both variables, PC2 was strongly correlated with unmanaged plots downslope and less correlated with croplands and upslope regions. For the variable 'nitrate content', this component was most sensitive to surface porosity (factor F), while for the variable 'ammonium uptake', PC2 was mostly affected by interaction terms;

vii. For both variables, PC3 exhibited more complex correlations with the landscape slope and the checkerboard distribution of croplands. For nitrate content, this component was mostly affected by interaction terms, while for ammonium uptake by plants, PC3 was mainly affected by the lateral transmissivity of soil.

In short, the detailed 2D-spread sensitivity analysis allowed assessing how each input factor affected the spatial distribution of each outcome variable averaged over time.
Figure 4: Spatial sensitivity analysis of nitrate concentration at a 60 cm depth. a) map of averages over time and over the factorial design. b) rsd: coefficient of variation between runs of the factorial design; c) map of the factors with the highest total sensitivity index (tSI) at each pixel; global sensitivity analysis: d-f) decomposition of the first three principal components; h-i) total sensitivity indexes of each factor on each PC, split into main effect (black) and interaction (gray) terms.
Figure 5: Spatial sensitivity analysis of cumulated ammonium uptake by plants. a) map of averages over time and over the factorial design. b) rsd: coefficient of variation between runs of the factorial design; c) map of the factors with the highest total sensitivity index (tSI) at each pixel; global sensitivity analysis: d-f) decomposition of the first three principal components; g-i) total sensitivity indexes of each factor on each PC, split into main effect (black) and interaction (gray) terms.
3.3 Correspondence between spatially explicit and dynamic sensitivity analyses

Figures 3 and 5 represent two different aspects of the detailed sensitivity analysis of the variable ‘ammonium uptake by plants’. The spatially explicit and the dynamic analyses allowed exploring the datasets from two complementary perspectives and offered a comprehensive visualization of the impact of each factor. For instance, the dynamic analysis showed that for the fertilization period, the most important factor throughout the whole landscape was the type of fertilizer. However, surface porosity took a predominant role later on. Meanwhile, it could be appreciated in the 2D map that the type of fertilizer had a greater effect upslope, but also that porosity was more important downslope. Both observations indicated that the amount of ammonium captured by plants was highly dependent on the percolation dynamics of the fertilizer.

A detailed analysis of how each factor affects each variable is beyond the scope of this paper.

3.4 Classification of the sensitivity indexes of the ensemble of outcomes

A cluster analysis was applied to the ensemble of sensitivity indexes resulting from the sensitivity analysis of all spatially- and temporally-aggregated outcomes, in order to group outcomes with similar response to input factors.

Figure 6 shows the clusters into which model outcomes were split. The number of clusters \( M = 5 \) was set as the minimal number providing equal classifications of the outcomes with different clustering algorithms (k-means and hierarchical clustering). This partitioning allowed explaining 73.6% of the variance of the sensitivity indexes and the number of clusters found this way corresponded to the number that would be chosen qualitatively with the elbow method (Ketchen and Shook, 1996).

The principal projections of the clusters of outcomes onto the axes of the transformed space are shown in Figures 7a, 7b and 7c. The corresponding principal projections of the sensitivity indexes of input factors onto the axes of the transformed space are shown in Figures 7d, 7e and 7f.

The projection PC1-PC2 explained 65.6% of the variance of the sensitivity indexes. This projection allowed a clear discrimination of clusters 1, 2 and 4, but clusters 3 and 5 were not so easily singled out (Figure 7f). This observed cluster separation was driven by the main effects of factors J, F and to a lesser extent C and D. Indeed, clusters were split along the axes indicated by the arrows corresponding to the main effect of these factors, the length of each arrow being proportional to the importance of each effect (Figure 7f). In these scheme, orthogonality indicates that indexes are independent from each other: the effects of J and F were almost independent from each other, as well as F, C and D. In contrast, J was antiparallel to C and D, indicating that whenever J had an effect, the other two did not, and vice versa. Finally, factors C and D were parallel to each other indicating that they had the same effect.
Figure 6: 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; gray line: SA results are expressed in terms of main effects of each factor and the ensemble of pairwise interaction terms $\Omega$ (pairwise SI); b) hierarchical clustering of outcomes: outcomes are linked together if they have similar profiles of sensitivity indexes; Inertia gain: variance explained when outcomes are linked together. Color 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. Colors of each line are set according to the colors of clusters.
Figure 7: Principal Component Analysis and clustering of the results of the global sensitivity indexes resulting from the analysis of all NitroScape outcomes. 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 same planes.
on the same clusters of variables.

The projection PC1-PC3 explained 62% of the variance. In these projection, cluster splitting was driven by the main effects of factors J, B and F (Figures 7b and 7e). Cluster 5 was separated along the axis of the main effect B, while cluster 2 could be singled out along the axis F, and in opposition to J. This meaning that variables in cluster were affected by the main effect of factor F and not by the main effect of J.

The projection PC2-PC3 explained 37.5% of the variance (Figures 7c and 7f). It allowed a clear discrimination of cluster 5 as well as splitting the other clusters along the axes of the main effects of factors C, D and F.

As it can be appreciated in Figure 7, the total amount of nitrogen in catchment discharge is always placed near the origin. This indicates that this variable was equally affected by the main effects and interactions of each factor appearing in the projections.

Table 2 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.

| Cluster | N | Outcomes                                                                 | Characteristics                                                                                                           |
|---------|---|---------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------|
| K=1     | 9 | Evapo-transpiration, Nitrogen emission and uptake by plants, Nitrogen mineralization, depth of the groundwater table and total amount of nitrogen in catchment discharge | Mostly affected by the soil lateral water transmissivity (factor C) and the decrease in soil transmissivity with depth (factor D). |
| K=2     | 5 | Total ammonium and nitrate concentration in catchment discharge, Nitrification, total amount of groundwater and ammonium concentration in groundwater | Mostly affected by the porosity of soil (factor F).                                                                          |
| K=3     | 7 | Surface water depths, Streaming flow and water catchment discharge, nitrogen adsorbed in soil microporosity, nitrate in groundwater | Mostly affected by the porosity of soil (factor F), type of fertilization (factor J), the soil lateral water transmissivity (factor C) and the decrease in soil transmissivity with depth (factor D). Moderate impact of interaction terms. |
| K=4     | 6 | Ammonium concentration in groundwater and in catchment discharge, nitrogen adsorbed in soil macroporosity, nitrate in superficial soil. | Mostly affected by the type of fertilization (factor J). High impact of the interaction term J:K. |
| K=5     | 2 | Ammonium in surface soil and nitrate concentration in groundwater          | Mostly affected by the vertical resolution of the model.                                                                  |

Some closing remarks regarding the analysis here presented are discussed next.

Clusters grouped variables that were sensitive to the same factors. However, this did not entail that these factors affected those variables in the same way: for example, $sNO_3(60cm)$ and $NH_4(GW)$ were grouped together in cluster 4 as they both had a high sensitivity to
the lateral transmissivity of soil (factor C), while $sNO_3(60cm)$ decreased and $NH_4(GW)$ increased with increasing C.

In broad terms, model outcomes were mostly affected by the hydrological characteristics of soil and management (i.e. type of fertilization). Interaction terms had significant effects on the detailed sensitivity analyses of every outcome, but they were less important for spatially- and temporally-aggregated outcome variables. The model resolution did have a significant effect on some model outcomes, comparable to the effect of other input factors. The horizontal resolution of the model (A) had a significant effect on several variables, but only for some regions of the landscape and not at the aggregated level. The vertical resolution (B) had a significant impact on two spatially- and temporally-aggregated variables: $sNH_4(60cm)$ and $NO_3(GW)$.

4 Conclusions

We developed a procedure to perform a comprehensive sensitivity analysis of a complex model with several scalar input factors and multiple spatially distributed and dynamic outcome variables. Then, we proposed a method to synthesize and visualize the ensemble of results of the sensitivity analyses. Some general conclusions regarding the applicability and generalization of the methods here presented are discussed below.

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 may be aggregated by land use, if pixels that hold a particular crop at a particular time are grouped together. Alternatively, data may be aggregated in function of the meteorological inputs, for instance by grouping together the days immediately after a rain event. These type of aggregations could be used to compare different types of agronomic management strategies or to design alternative managing responses to meteorology.

The detailed spatial and dynamic sensitivity analyses of each model outcome were here presented for just two sample outcomes, but every other outcome of the model has been thoroughly characterized in the same way. Given that the purpose of this paper is to present some methodological tools, the synthesis and visualization of the sensitivity indexes of the ensemble of factors on the ensemble of outcomes was here applied only to spatially- and temporally-aggregated outcome variables. This synthesis may be easily extended to any set of outcomes characterized by any set of sensitivity indexes, in particular, by those resulting from other types of aggregated variables.

Our results provided a thorough characterization of each outcome variable. The synthesis of these results permitted the classification of outcomes based on their responses to the ensemble of input parameters, as well as the classification of input parameters based on their influence on the ensemble of outcomes. In particular, our methods indicated that spatial resolution does have an impact on the outcomes of the model. Finally, the presented methods may be used for dimensionality reduction of the input space, because they allow ruling out
parameters that have nearly no influence on the outcomes within the range of explored values and in this virtual scenario: such as the ratio of microporosity to macroporosity of the soil, or the depth of the intermediate soil layer.

Nevertheless, the extrapolation of the obtained results to specific real settings is not straightforward, as the comparison between the effects of the spatial resolution of the simulator and the accuracy of sampled real-world observations were beyond the scope of the current work.

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References

Bishop, T. and Lark, R. (2006). The geostatistical analysis of experiments at the landscape-scale. Geoderma, 133(1):87–106.

Chen, H. H. and Cheng, C.-S. (2011). Fractional factorial designs. Design and Analysis of Experiments, Special Designs and Applications, 3:299.

Drouet, J.-L., Capian, N., Fiorelli, J.-L., Blanfort, V., Capitaine, M., Duretz, S., Gabrielle, B., Martin, R., Lardy, R., Cellier, P., et al. (2011). Sensitivity analysis for models of greenhouse gas emissions at farm level. Case study of N2O emissions simulated by the CERES-EGC model. Environmental Pollution, 159(11):3156–3161.

Duretz, S., Drouet, J.-L., Durand, P., Hutchings, N. J., Theobald, M., Salmon-Monviola, J., Dragosits, U., Maury, O., Sutton, M., and Cellier, P. (2011). NitroScape: a model to integrate nitrogen transfers and transformations in rural landscapes. Environmental Pollution, 159(11):3162–3170.

Faivre, R., Iooss, B., Mahévas, S., Makowski, D., and Monod, H. (2013). Analyse de sensibilité et exploration de modèles: application aux sciences de la nature et de l’environnement. Editions Quae.

Galloway, J. N., Aber, J. D., Erisman, J. W., Seitzinger, S. P., Howarth, R. W., Cowling, E. B., and Cosby, B. J. (2003). The nitrogen cascade. Bioscience, 53(4):341–356.

Kaufman, L. and Rousseeuw, P. J. (2009). Finding groups in data: an introduction to cluster analysis, volume 344. John Wiley & Sons.
Ketchen, D. J. and Shook, C. L. (1996). The application of cluster analysis in strategic management research: an analysis and critique. *Strategic management journal*, 17(6):441–458.

Kobilinsky, A., Bouvier, A., and Monod, H. (2012). Planor: an r package for the automatic generation of regular fractional factorial designs. Technical report, Citeseer.

Lamboni, M., Makowski, D., Lehuger, S., Gabrielle, B., and Monod, H. (2009). Multivariate global sensitivity analysis for dynamic crop models. *Field Crops Research*, 113(3):312–320.

Lamboni, M., Monod, H., and Makowski, D. (2011). Multivariate sensitivity analysis to measure global contribution of input factors in dynamic models. *Reliability Engineering & System Safety*, 96(4):450–459.

Lê, S., Josse, J., Husson, F., et al. (2008). Factominer: an r package for multivariate analysis. *Journal of statistical software*, 25(1):1–18.

Ligmann-Zielinska, A. (2013). Spatially-explicit sensitivity analysis of an agent-based model of land use change. *International Journal of Geographical Information Science*, 27(9):1764–1781.

Marrel, A., Iooss, B., Jullien, M., Laurent, B., and Volkova, E. (2011). Global sensitivity analysis for models with spatially dependent outputs. *Environmetrics*, 22(3):383–397.

Moreau, P., Viaud, V., Parnaudeau, V., Salmon-Monviola, J., and Durand, P. (2013). An approach for global sensitivity analysis of a complex environmental model to spatial inputs and parameters: A case study of an agro-hydrological model. *Environmental modelling & software*, 47:74–87.

Morris, M. D. (1991). Factorial sampling plans for preliminary computational experiments. *Technometrics*, 33(2):161–174.

Suzuki, R. and Shimodaira, H. (2006). Pyclust: an r package for assessing the uncertainty in hierarchical clustering. *Bioinformatics*, 22(12):1540–1542.