

MoSAR Systemic modelling applied to ruminants

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To whom it may concern

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Implementation of a dynamic sensitivity analysis of a mathematical model describing the effect of the macroalgae *Asparagopsis taxiformis* on rumen fermentation and methane production under *in vitro* continuous conditions

Agreement with INRAE

Dear colleague,

Thanks for your interest in our work. The set of R files you have received contain the implementation of a dynamic sensitivity analysis of a mathematical model of rumen *in vitro* continuous fermentation accounting for the impact of *Asparagopsis taxiformis* supply on the fermentation and methane production. It is composed of 3 folders: 1) the implementation of the mathematical model, 2) the implementation of the Shapley effects and 3) the implementation of the the full and independent Sobol indices.

The files of the model implementation are:

DynamicIntake: function simulating the dynamic intake.

rumencATload: file to load the initial conditions of the model, simulate the dynamic intake and set the parameters of dietary scenarios.

rumencAT: function where the ordinary differential equation system is defined.

rumencATplot: function to run the simulation of the model. It plots the model outputs and compare the simulations of the 3 dietary scenarios.

rumencATout: auxiliary function to select the output variables studied in the sensitivity analysis.

The files of the Shapley effects implementation are:

InputparamSamplingmat: file to simulate the sampling matrix of input parameters used to compute the Shapley effects.

FunctionsShapleyeffects: functions for computing the Shapley effects (R package sensitivity).

ModelOutputsCompDietChagasControl: file computing the output variables of the *Asparagopsis taxiformis* model for the control using the sampling matrix of input parameters simulated.

ModelOutputsCompDietChagasLow: file computing the output variables of the *Asparagopsis taxiformis* model for the low *Asparagopsis taxiformis* treatment using the sampling matrix of input parameters simulated.

ModelOutputsCompDietChagasHigh: file computing the output variables of the *Asparagopsis taxiformis* model for the high *Asparagopsis taxiformis* treatment using the sampling matrix of input parameters simulated.

ShapleyeffectsCompDietChagasControl: file computing the Shapley effects for the 4 output variables of the *Asparagopsis taxiformis* model studied for the control.

ShapleyeffectsCompDietChagasLow: file computing the Shapley effects for the 4 output variables of the *Asparagopsis taxiformis* model studied for the low *Asparagopsis taxiformis* treatment.

ShapleyeffectsCompDietChagasHigh: file computing the Shapley effects for the 4 output variables of the *Asparagopsis taxiformis* model studied for the high *Asparagopsis taxiformis* treatment.

ShapleyeffectsPlot: file plotting the dynamic of Shapley effects and performing the uncertainty analysis of output variables simulated.

The files of the full and independent Sobol indices implementation are:

InputparamSamplingmat: file to simulate the sampling matrix of input parameters used to compute the full and independent Sobol indices.

BootstrapimplementationFunctions: functions for implementing the bootstrap replication when computing the Sobol indices (R package boot).

PickandFreezeStratFunctions: functions for implementing the “pick and freeze” strategy when computing the Sobol indices (R package sensobol).

SobolindicesCompFunctions: functions for computing the full and independent Sobol indices (R package sensobol).

ModelOutputsCompDietChagasControl: file computing the output variables of the *Asparagopsis taxiformis* model for the control using the sampling matrix of input parameters simulated.

ModelOutputsCompDietChagasLow: file computing the output variables of the *Asparagopsis taxiformis* model for the low *Asparagopsis taxiformis* treatment using the sampling matrix of input parameters simulated.

ModelOutputsCompDietChagasHigh: file computing the output variables of the *Asparagopsis taxiformis* model for the high *Asparagopsis taxiformis* treatment using the sampling matrix of input parameters simulated.

SobolindicesCompDietChagasControl: file computing the Sobol indices for the 4 output variables of the *Asparagopsis taxiformis* model studied for the control.

SobolindicesCompDietChagasLow: file computing the Sobol indices for the 4 output variables of the *Asparagopsis taxiformis* model studied for the low *Asparagopsis taxiformis* treatment.

SobolindicesCompDietChagasHigh: file computing the Sobol indices for the 4 output variables of the *Asparagopsis taxiformis* model studied for the high *Asparagopsis taxiformis* treatment.

SobolindicesPlot: file plotting the dynamic of Sobol indices.

These implementations are freely available for academic purposes to foster scientific exchange. The use of the codes for non-academic use is forbidden. By requesting them, you are accepting that you will not use it with any commercial application or in any work related with companies.

Please feel free to contact us if you have any query about the model and sensitivity analysis implementations. We will do our best to find the time to discuss. If you use our work in your research and publications, please acknowledge our work by citing our work.

We hope our developments will be useful for your work. Our main interest of rendering the code available is to favor academic exchange. You are very welcome to contact us to look for potential collaborations.

Sincerely,

A handwritten signature in black ink, appearing to be 'PB', with a long horizontal stroke extending to the right.