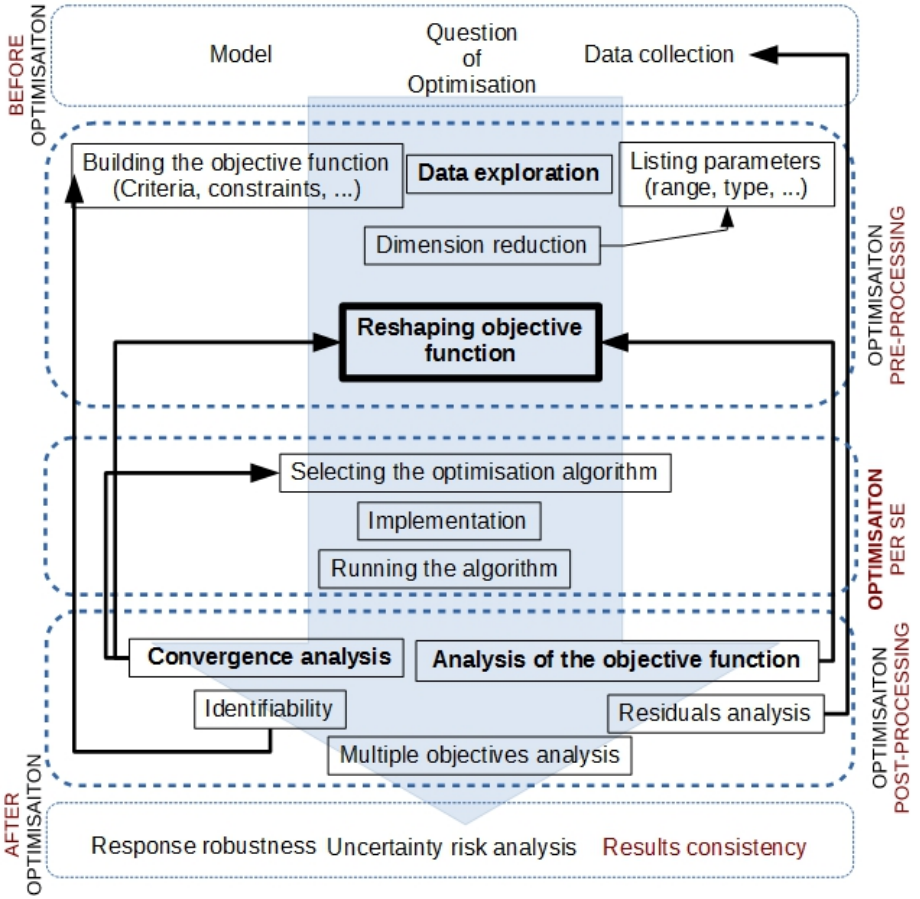
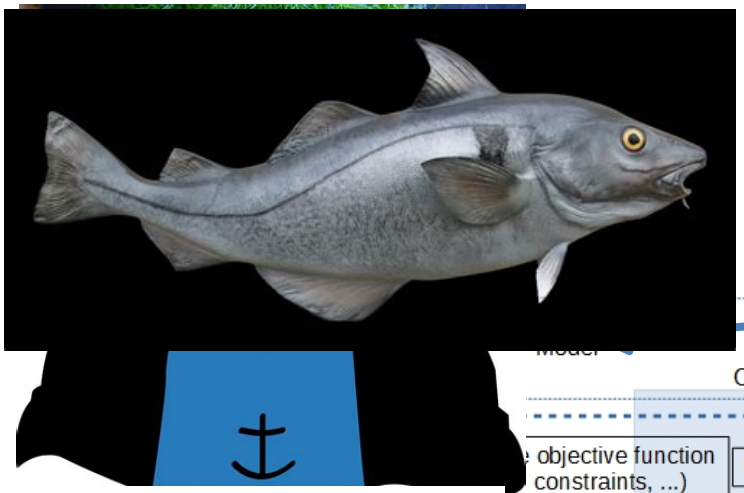
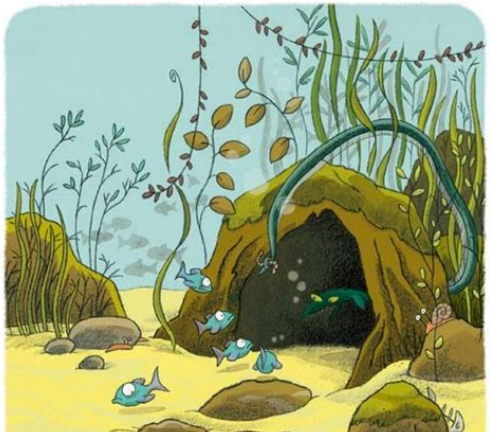
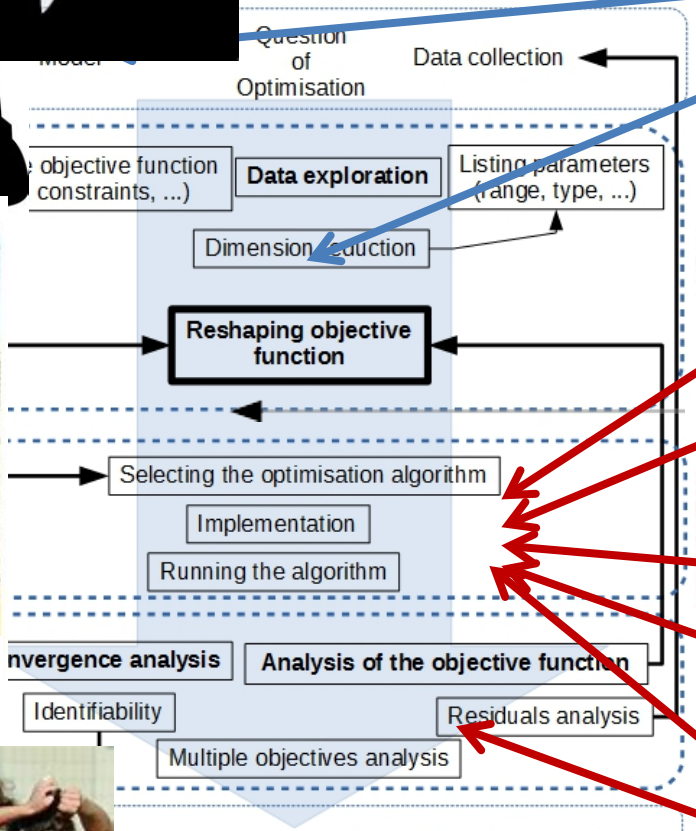
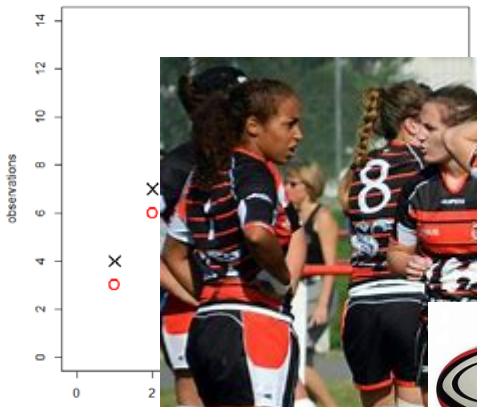
MEOW'18 : Mexico Easter Optimisation Workshop 2018











Analyses de sensibilité

Processus gaussien

Calibration Bayésienne

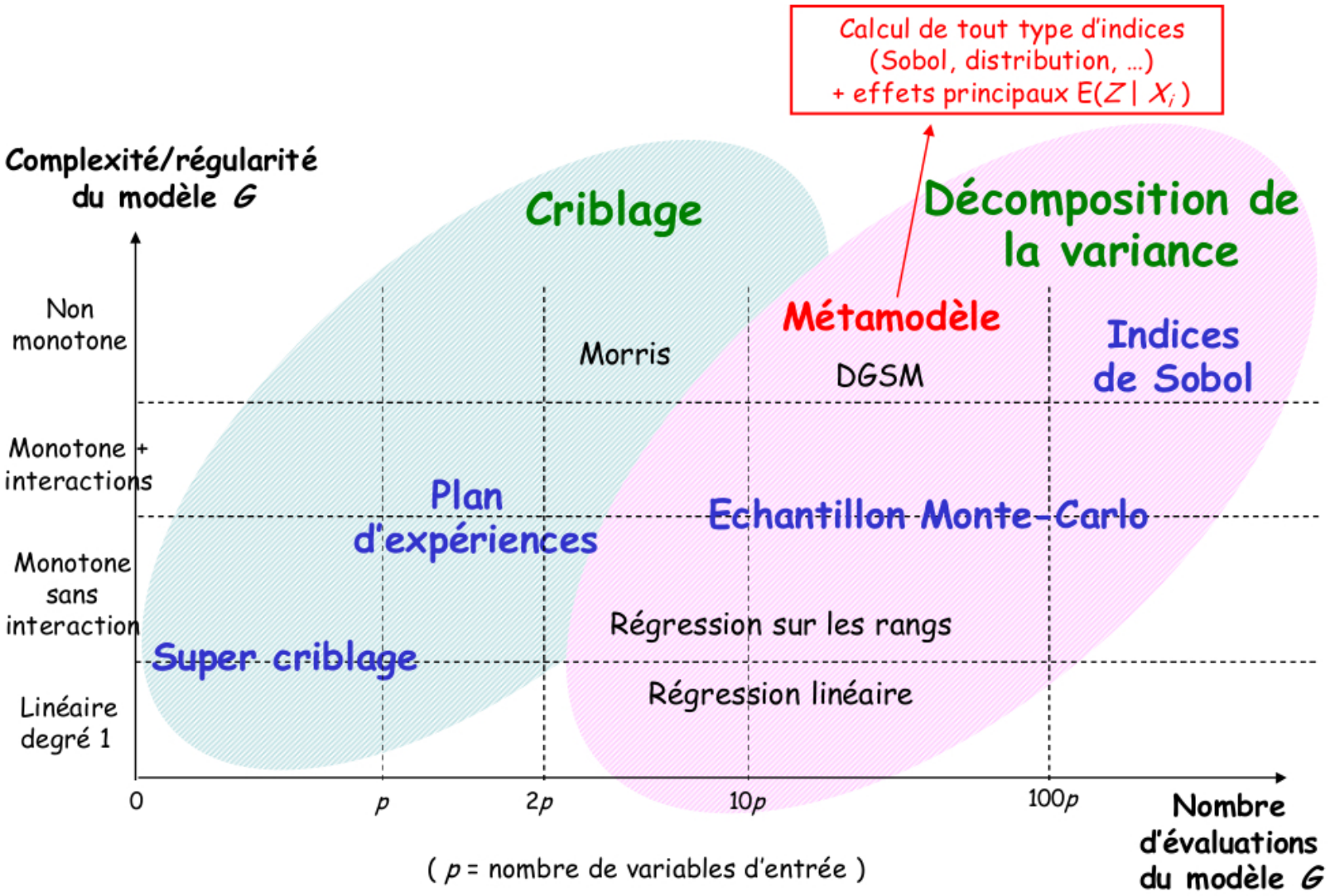
Algorithmes avec meta-modèle

Algorithmes sans meta-modèle

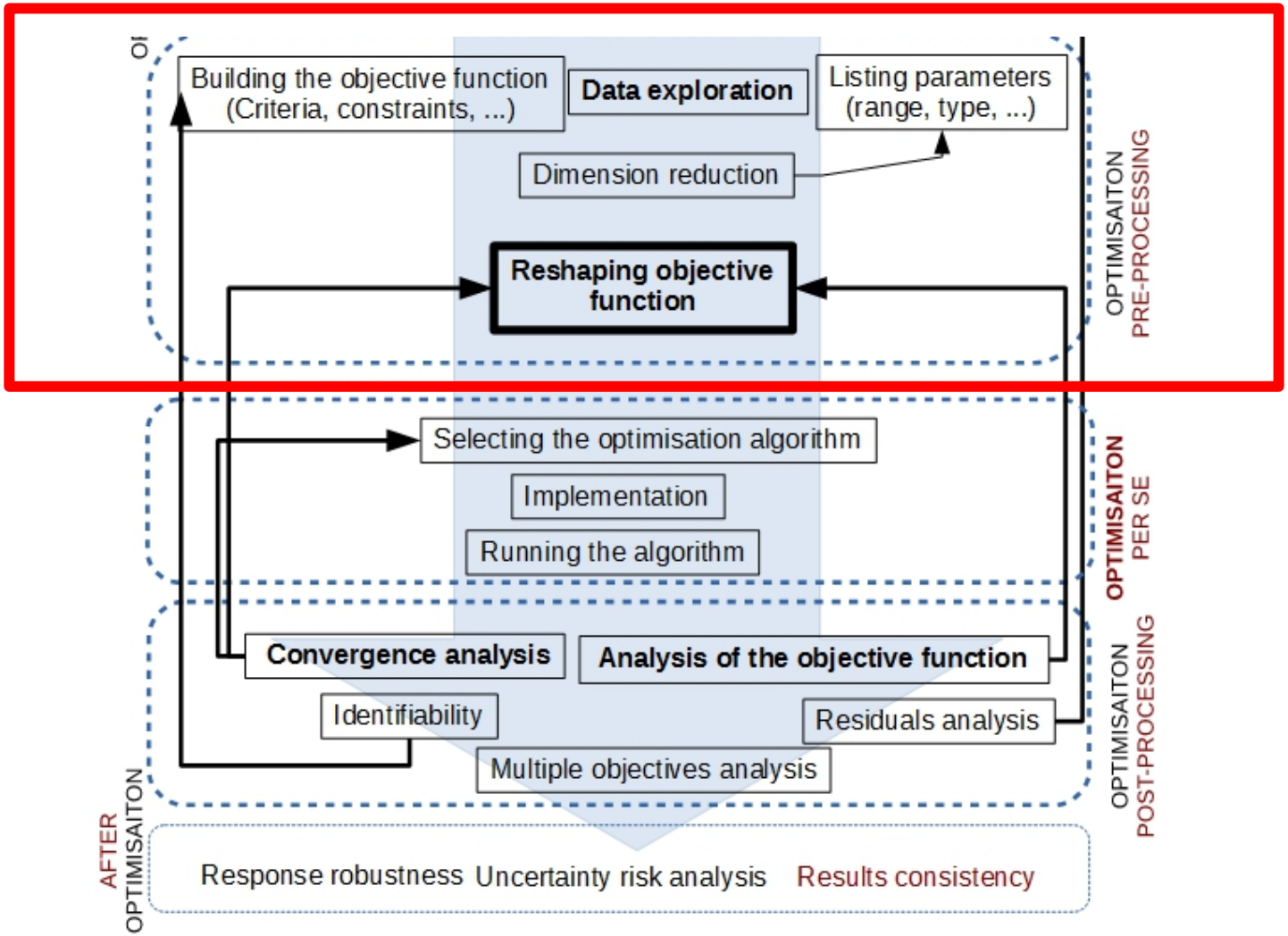
BC

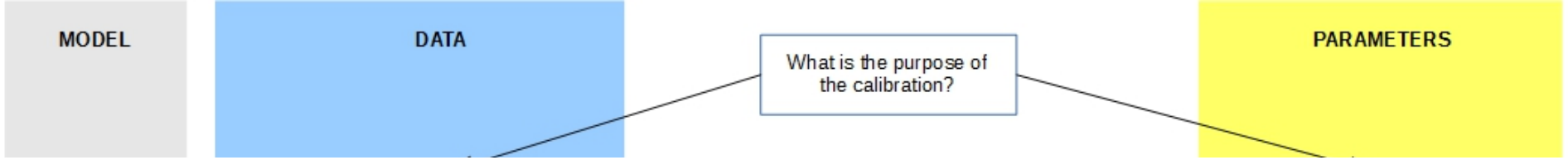
Multi-
es

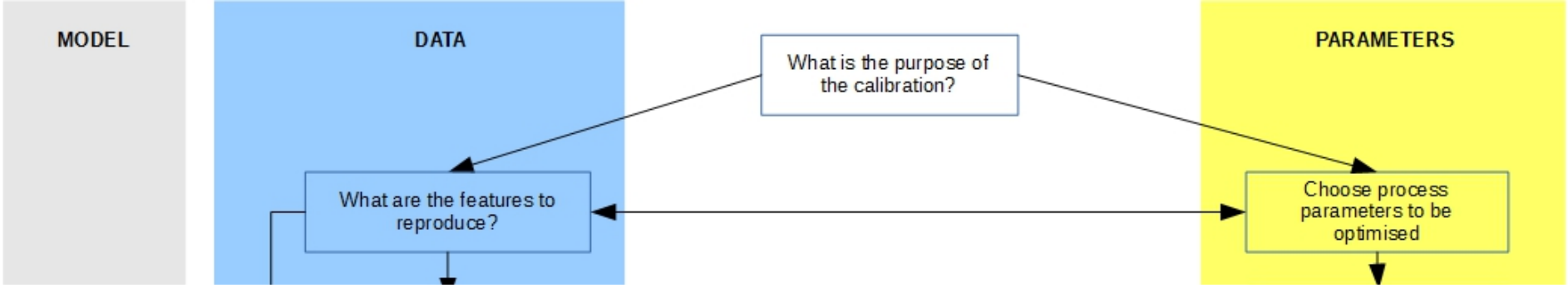
Classification des méthodes d'analyses de sensibilité

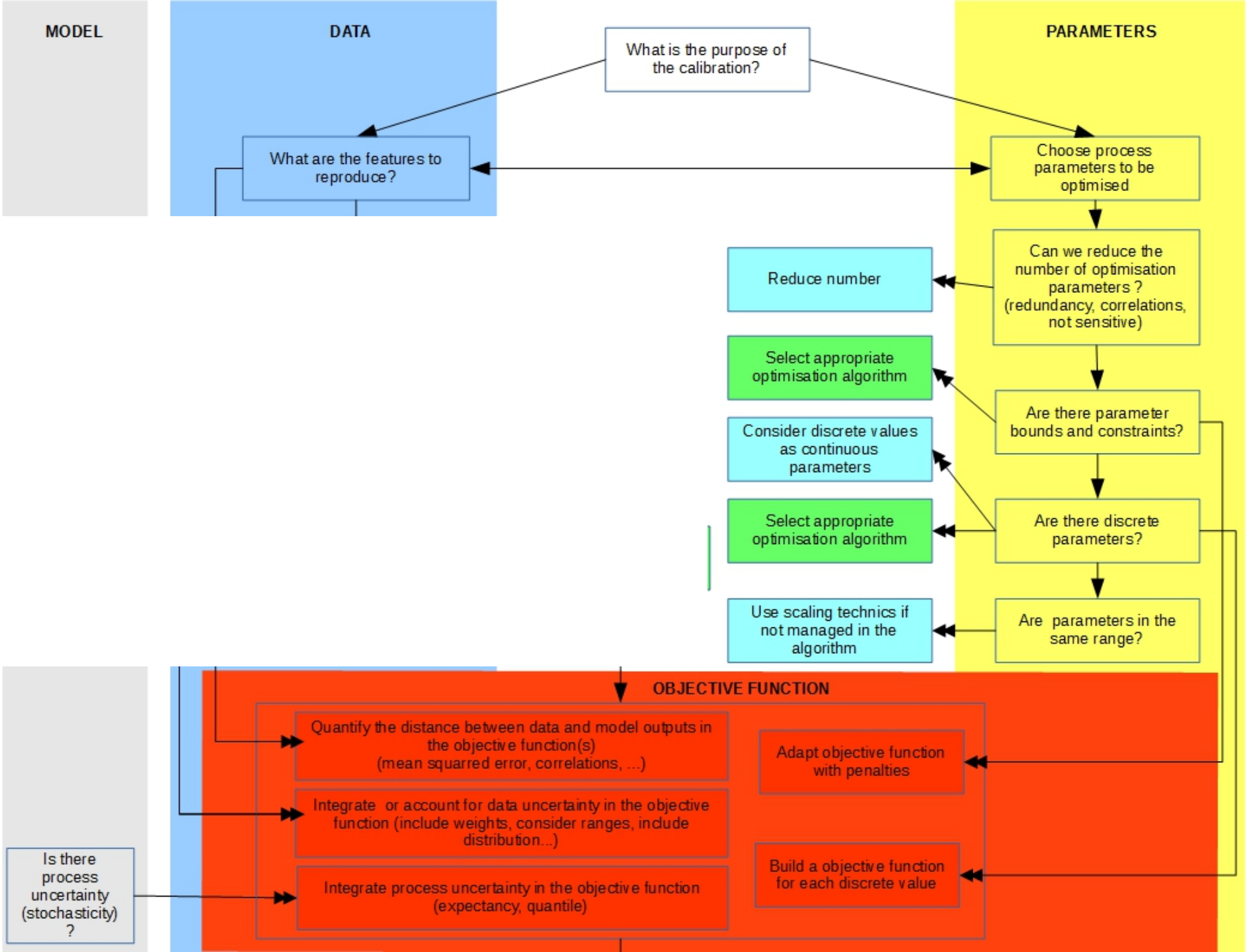


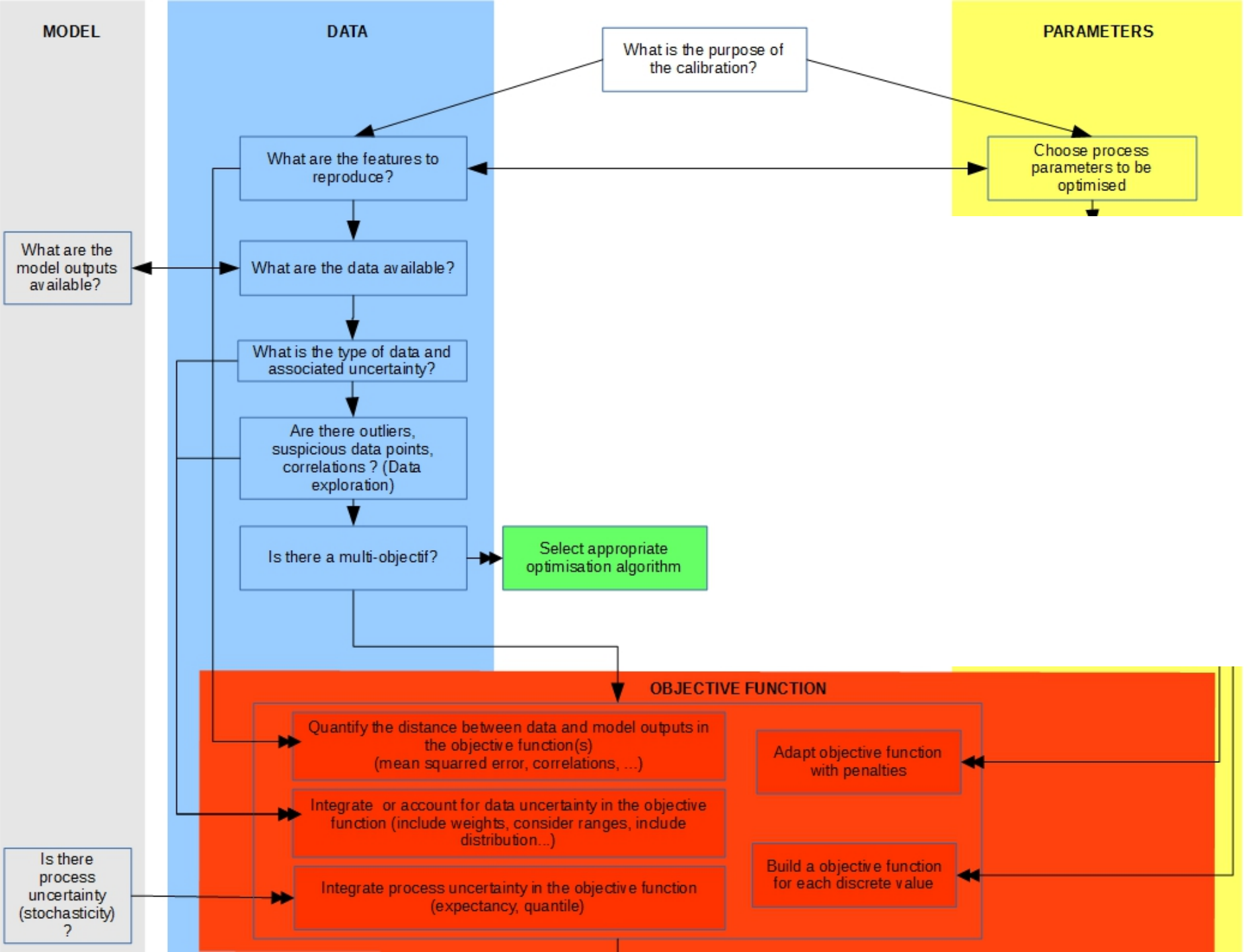
Pre-processing




MODEL
DATA
What is the purpose of the calibration?
PARAMETERS


MODEL
DATA
PARAMETERS
What is the purpose of the calibration?
What are the features to reproduce?
Choose process parameters to be optimised


MODEL
DATA
PARAMETERS
What is the purpose of the calibration?
What are the features to reproduce?
Choose process parameters to be optimised
Can we reduce the number of optimisation parameters ? (redundancy, correlations, not sensitive)
Reduce number
Are there parameter bounds and constraints?
Select appropriate optimisation algorithm
Consider discrete values as continuous parameters
Are there discrete parameters?
Select appropriate optimisation algorithm
Are parameters in the same range?
Use scaling technics if not managed in the algorithm
OBJECTIVE FUNCTION
Quantify the distance between data and model outputs in the objective function(s) (mean squarred error, correlations, ...)
Adapt objective function with penalties
Integrate or account for data uncertainty in the objective function (include weights, consider ranges, include distribution...)
Build a objective function for each discrete value
Integrate process uncertainty in the objective function (expectancy, quantile)
Is there process uncertainty (stochasticity) ?


MODEL
DATA
PARAMETERS
What is the purpose of the calibration?
What are the features to reproduce?
Choose process parameters to be optimised
What are the model outputs available?
What are the data available?
What is the type of data and associated uncertainty?
Are there outliers, suspicious data points, correlations ? (Data exploration)
Is there a multi-objectif?
Select appropriate optimisation algorithm
OBJECTIVE FUNCTION
Quantify the distance between data and model outputs in the objective function(s) (mean squarred error, correlations, ...)
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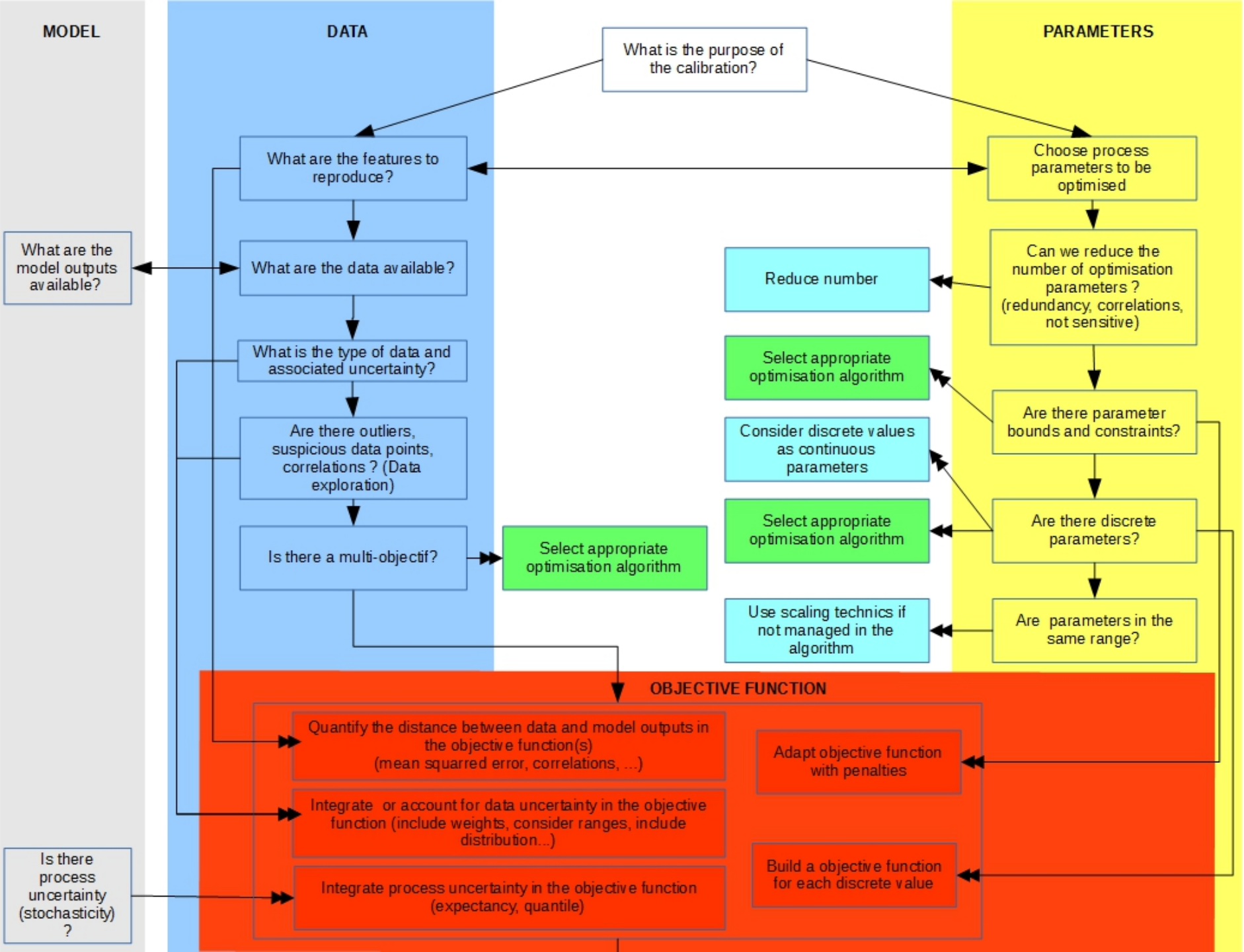
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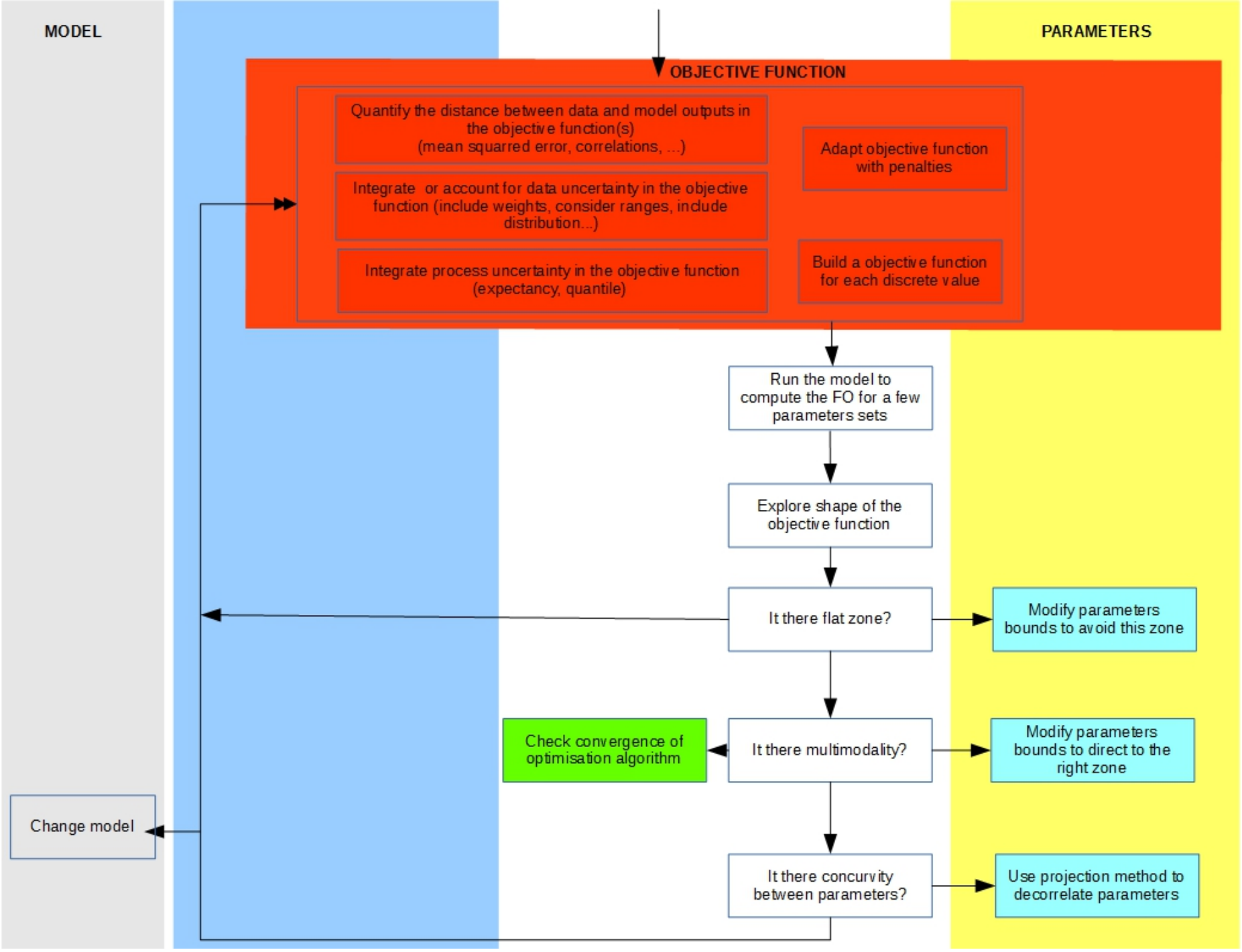
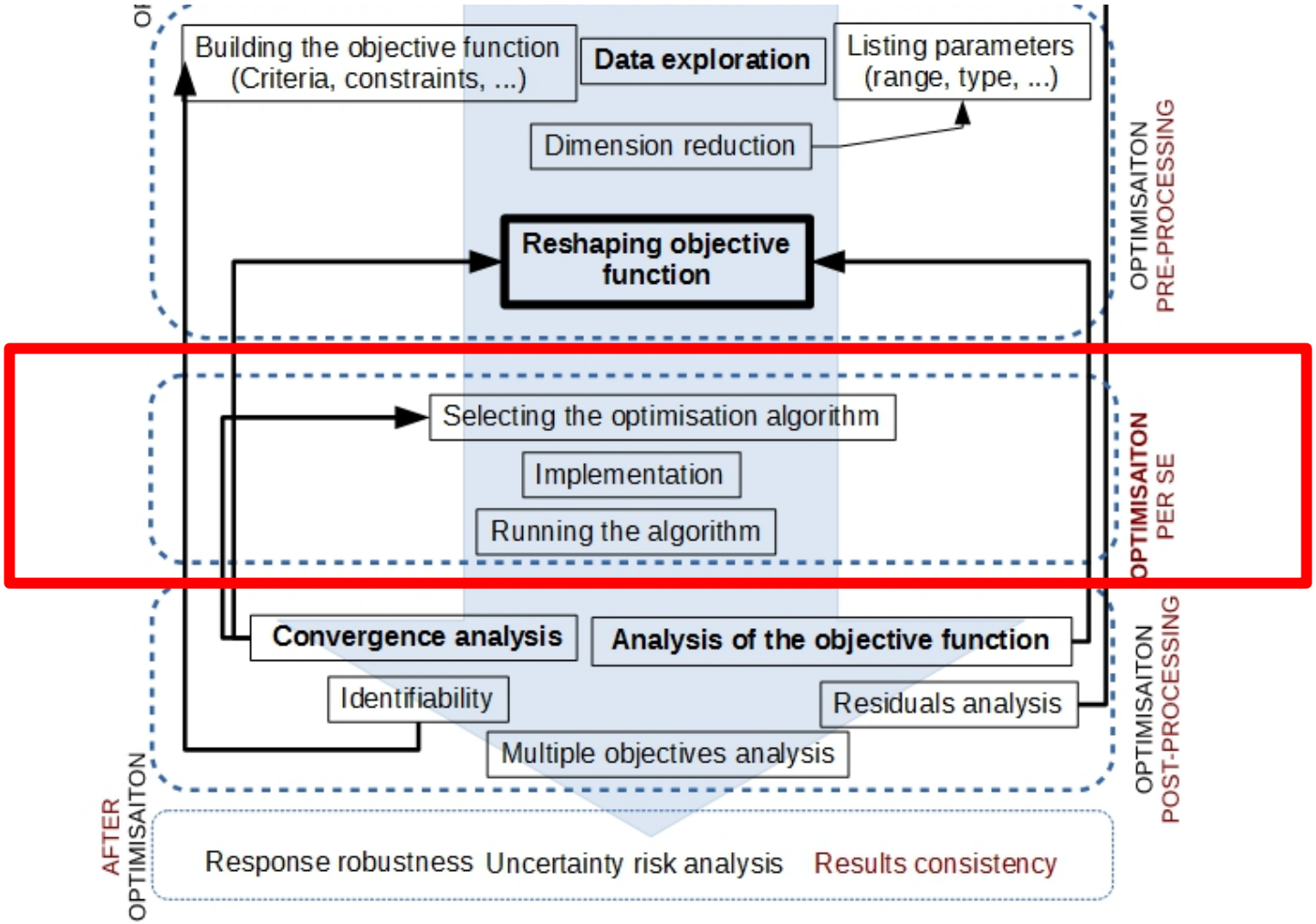
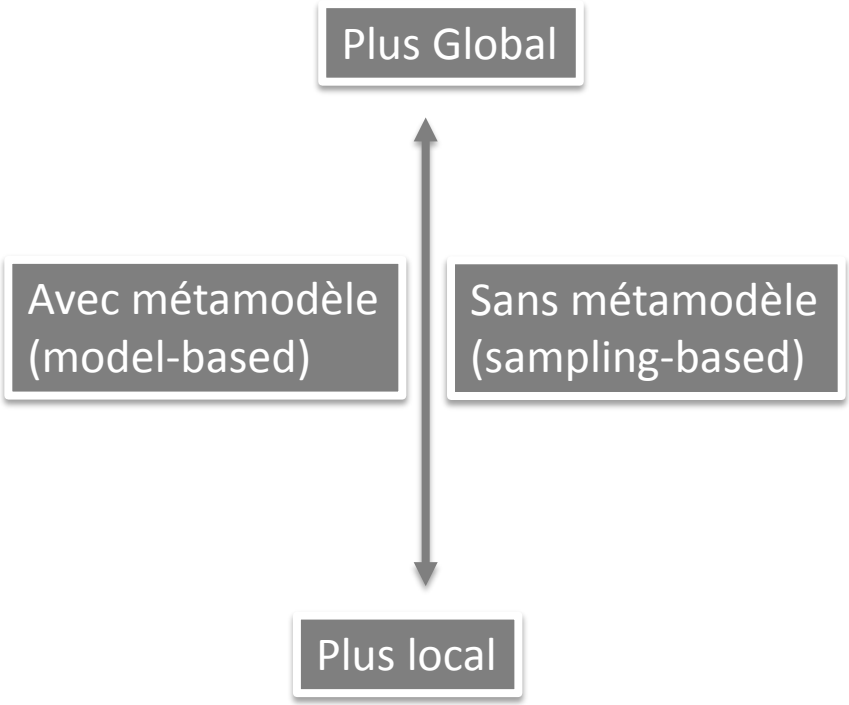

MODEL
PARAMETERS
OBJECTIVE FUNCTION
Quantify the distance between data and model outputs in the objective function(s) (mean squarred error, correlations, ...)
Integrate or account for data uncertainty in the objective function (include weights, consider ranges, include distribution...)
Integrate process uncertainty in the objective function (expectancy, quantile)
Adapt objective function with penalties
Build a objective function for each discrete value
Run the model to compute the FO for a few parameters sets
Explore shape of the objective function
It there flat zone?
Modify parameters bounds to avoid this zone
It there multimodality?
Check convergence of optimisation algorithm
Modify parameters bounds to direct to the right zone
It there concurvity between parameters?
Use projection method to decorrelate parameters
Change model

Algorithme

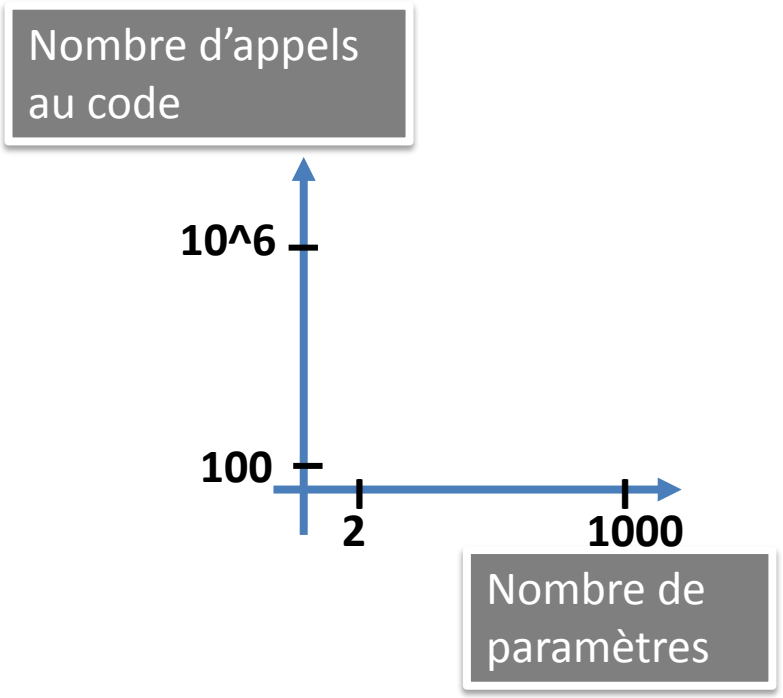

Building the objective function (Criteria, constraints, ...)
Data exploration
Listing parameters (range, type, ...)
Dimension reduction
Reshaping objective function
OPTIMISAITON PRE-PROCESSING
Selecting the optimisation algorithm
Implementation
Running the algorithm
OPTIMISAITON PER SE
Convergence analysis
Analysis of the objective function
Identifiability
Residuals analysis
Multiple objectives analysis
OPTIMISAITON POST-PROCESSING
AFTER OPTIMISAITON
Response robustness
Uncertainty risk analysis
Results consistency

Deux grilles pour guider la sélection

Grille 1 : Espace de projection



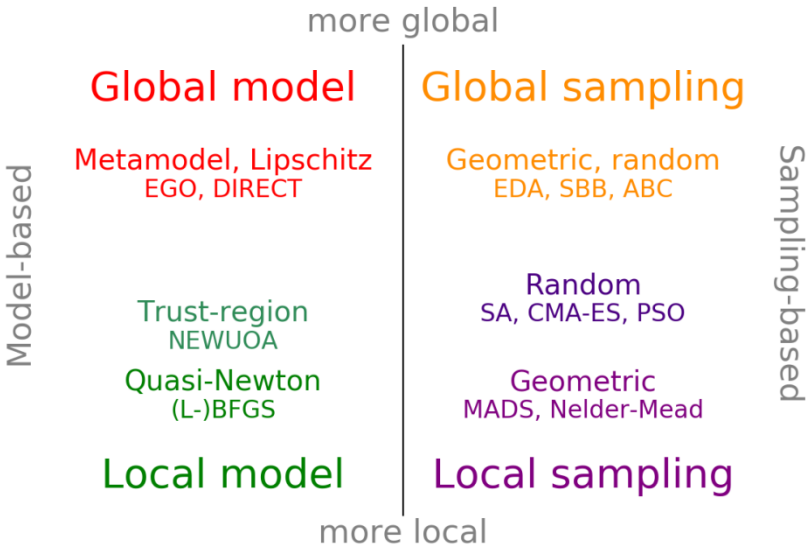
Grille 2: Aide à la sélection



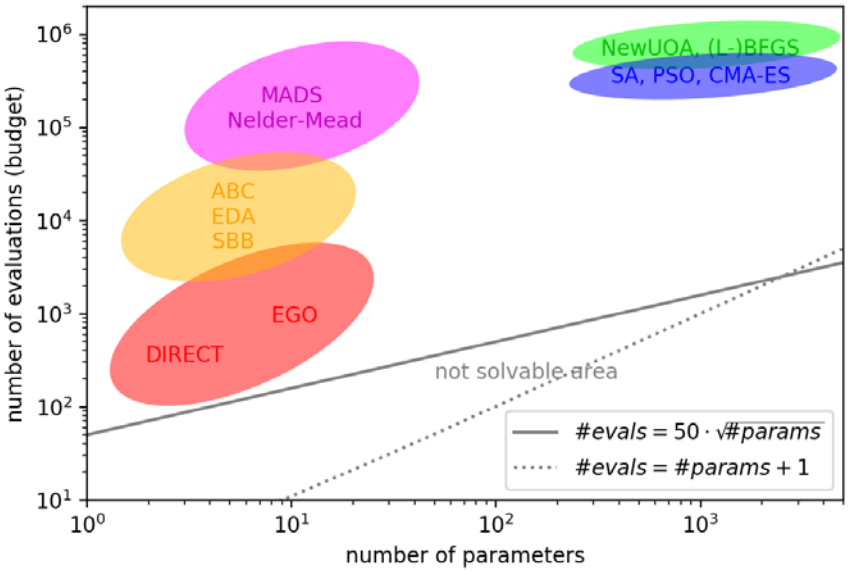
- **Grille 1 : positionner les différentes familles dans l'espace des deux critères**
- **Grille 2 : aider au choix de la famille d'optimisation**

Deux grilles pour guider la sélection

Grille 1 : Espace de projection



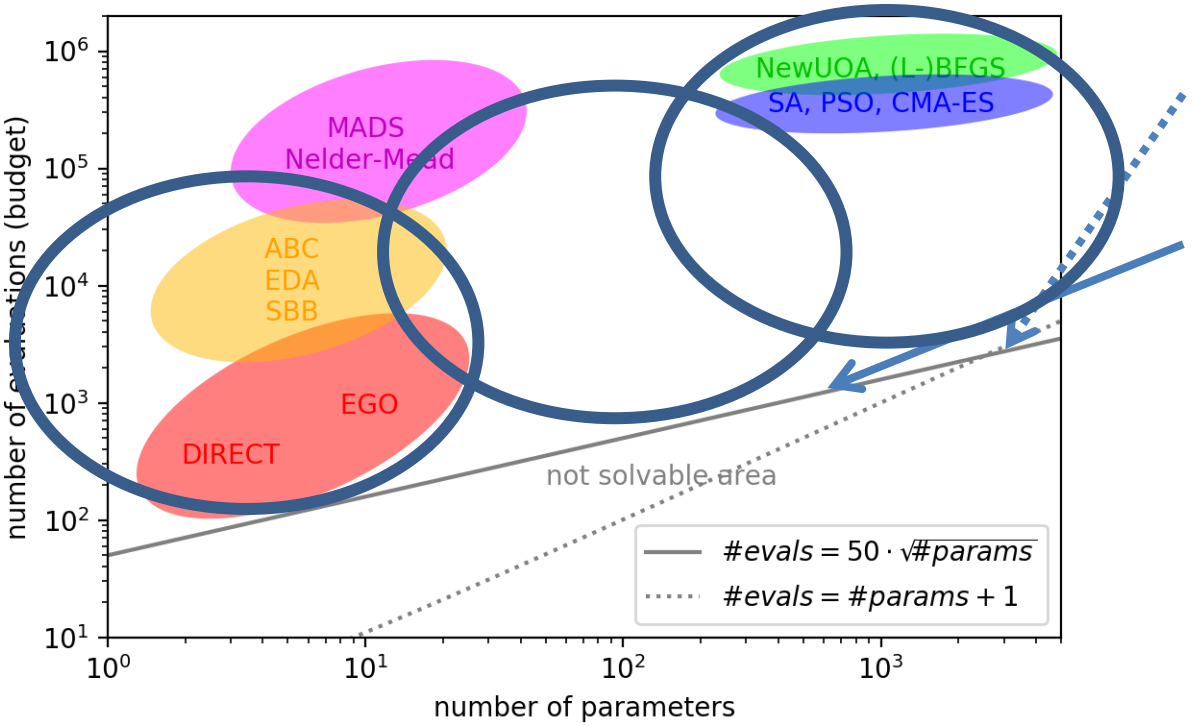
Grille 2: Aide à la sélection



- **Grille 1 : positionner les différentes familles dans l'espace des deux critères**
- **Grille 2 : aider au choix de la famille d'optimisation**

Stéphanie Mahévas[1], Victor Picheny[2], Patrick Lambert[3], Nicolas Dumoulin[4], Lauriane Rouan[5], Jean-Christophe Soulié[6], Dimo Brockhoff[7], Sigrid Lehuta[1], Rodolphe Le Riche[8], Robert Faivre[2], Hilaire Drouineau· Follow the guide! A handbook for conducting optimisation with complex ecological models based on feedback from practitioners. In Prep.

Grille : Paramètres/nombre d'évaluations



Problème linéaire non solvable

En général problème d'optimisation non solvable

Qui peut le plus peut le moins

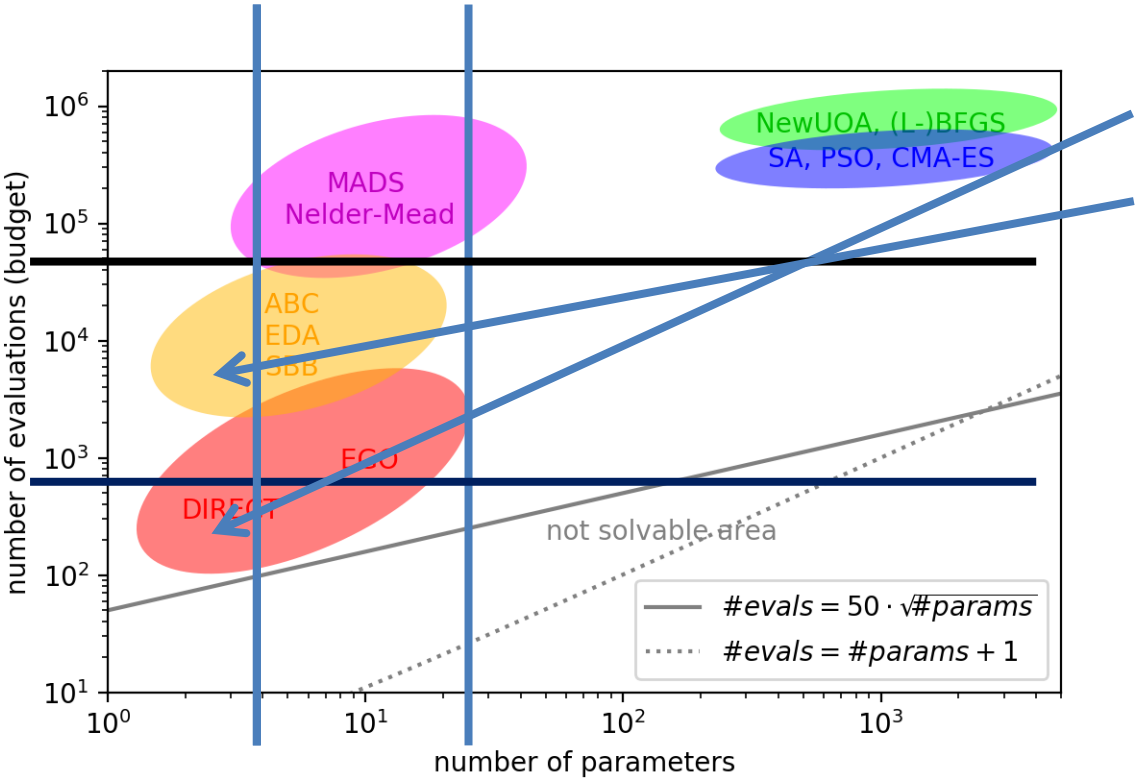
EGO : efficient global optimisation - Jones et al. (1998)
DIRECT : Dividing RECTangles – Jones et al 1993

NEWUOA : (Powell 2006)
L-BFGS-B : extension of Broyden-Fletcher-Goldfarb-Shanno 1987

EDA : Estimationof Distribution Algorithms (Larranag and Loranzo 2001)
SBB : Spatial Branch and Bound (Horst a,d Tuy 2013)
ABC Approximate Bayesian Computation (Csillery et al 2010)

SA : Simulated Annealing – recuit simule (Van Laarhoven et al 1987)
CMA-ES :Covariance Matrix Adaptation Evolution Strategy (Hansen et al 2003)
PSO : Particle swarn optimisation (Kennedy 2011)
MADS : Mesh Adaptative Direct Search (Audet et al 2006)
Nelder-Mead (Nelder et al 1965)

Grille : Paramètres/nombre d'évaluations



Peu de paramètres, peu de budget

Peu de paramètres, plus de budget

Plus de paramètres

EGO : efficient global optimisation - Jones et al. (1998)
DIRECT : Dividing RECTangles – Jones et al 1993

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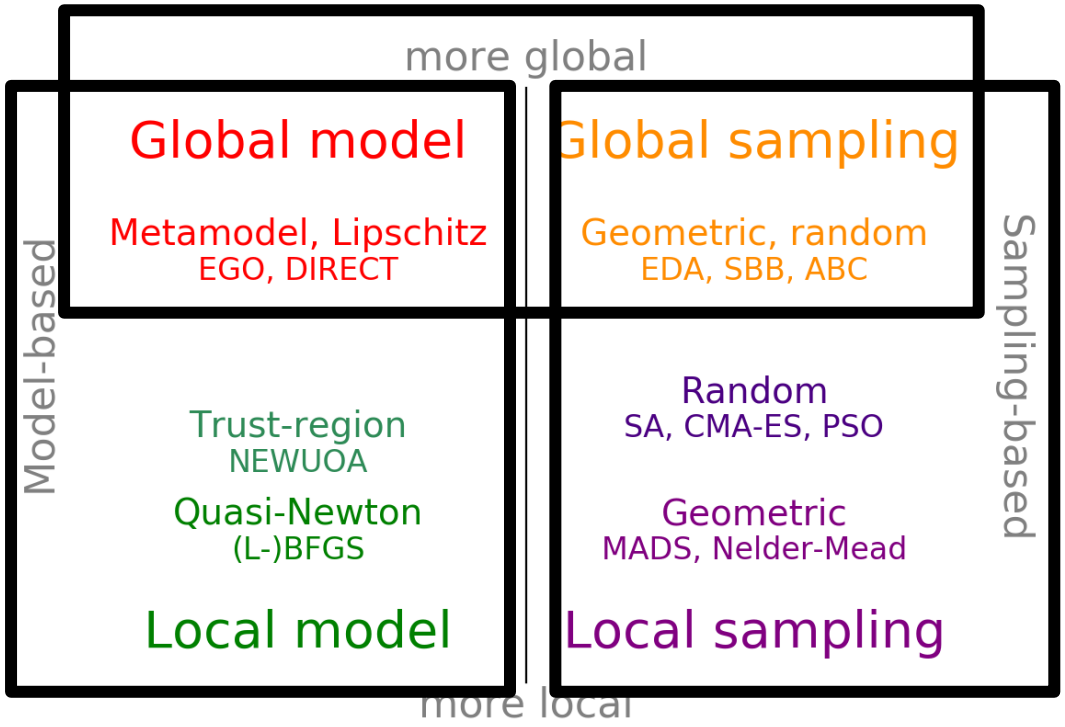
Grille : Recherche/métamodèle

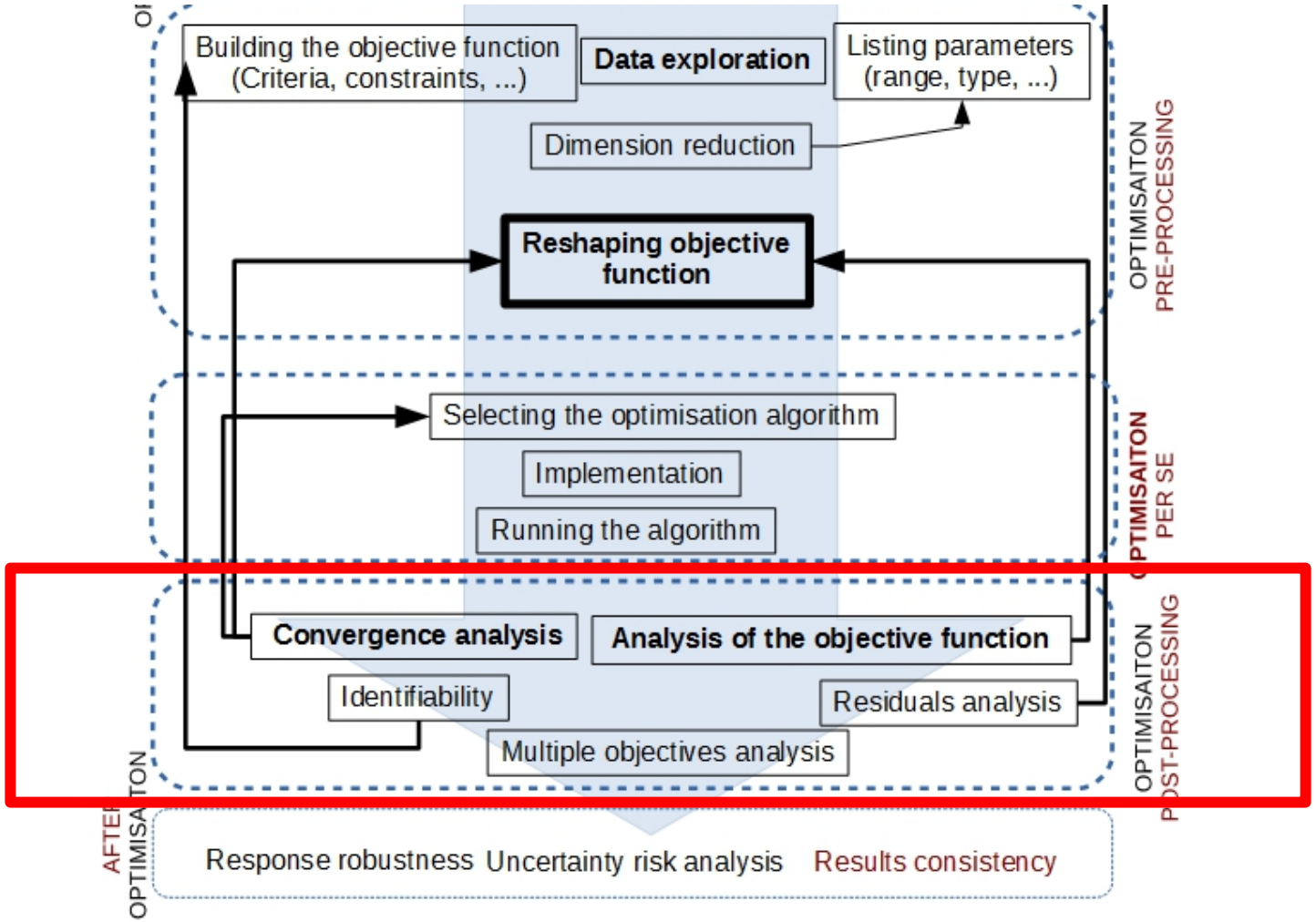


- Algorithmes de recherche globale : forme approchée de la fonction d'objectif sur l'espace des variables (la précision dépendra de l'équilibre entre la phase d'exploration et celle d'intensification)

- **Algorithmes avec métamodèle:** dérivées de premier et second ordre de la fonction autour de l'optimum (optimum ?, identifiabilité ?, intervalles de confiance ?)

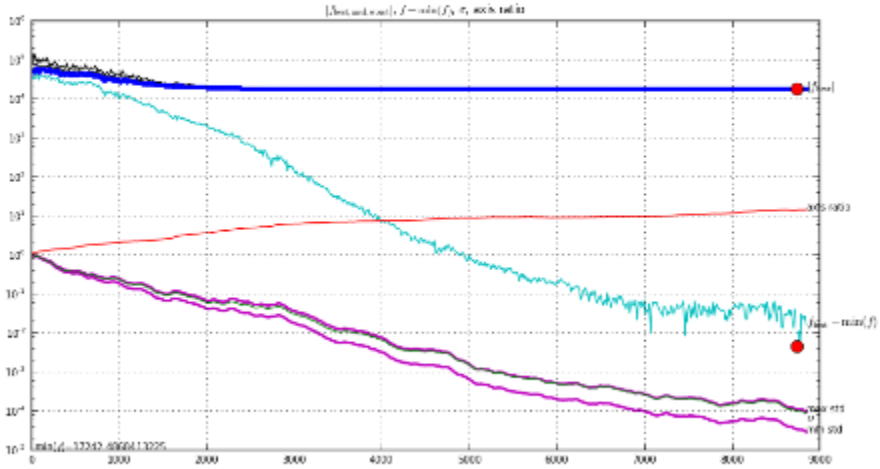
- **Algorithmes sans métamodèle :** famille de solutions autour de l'optimum (approcher la forme de la fonction d'objectif et des covariances des paramètres, distribution …)

Post-processing

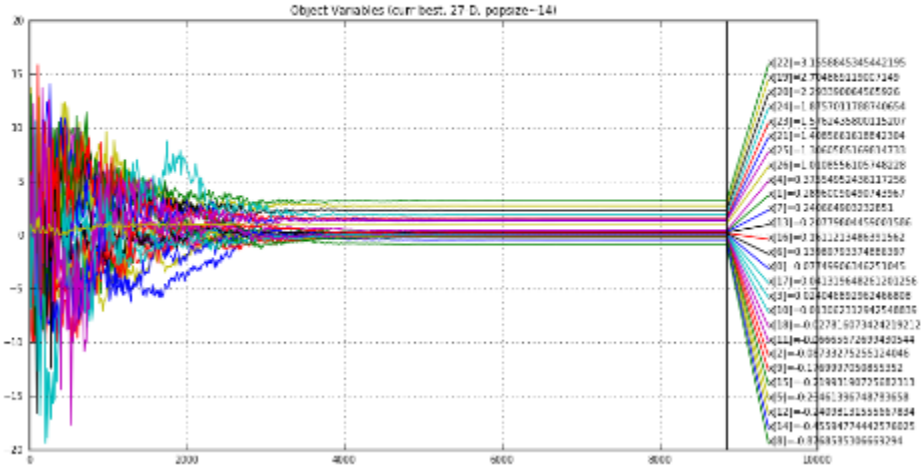


Traces

Espace objectif

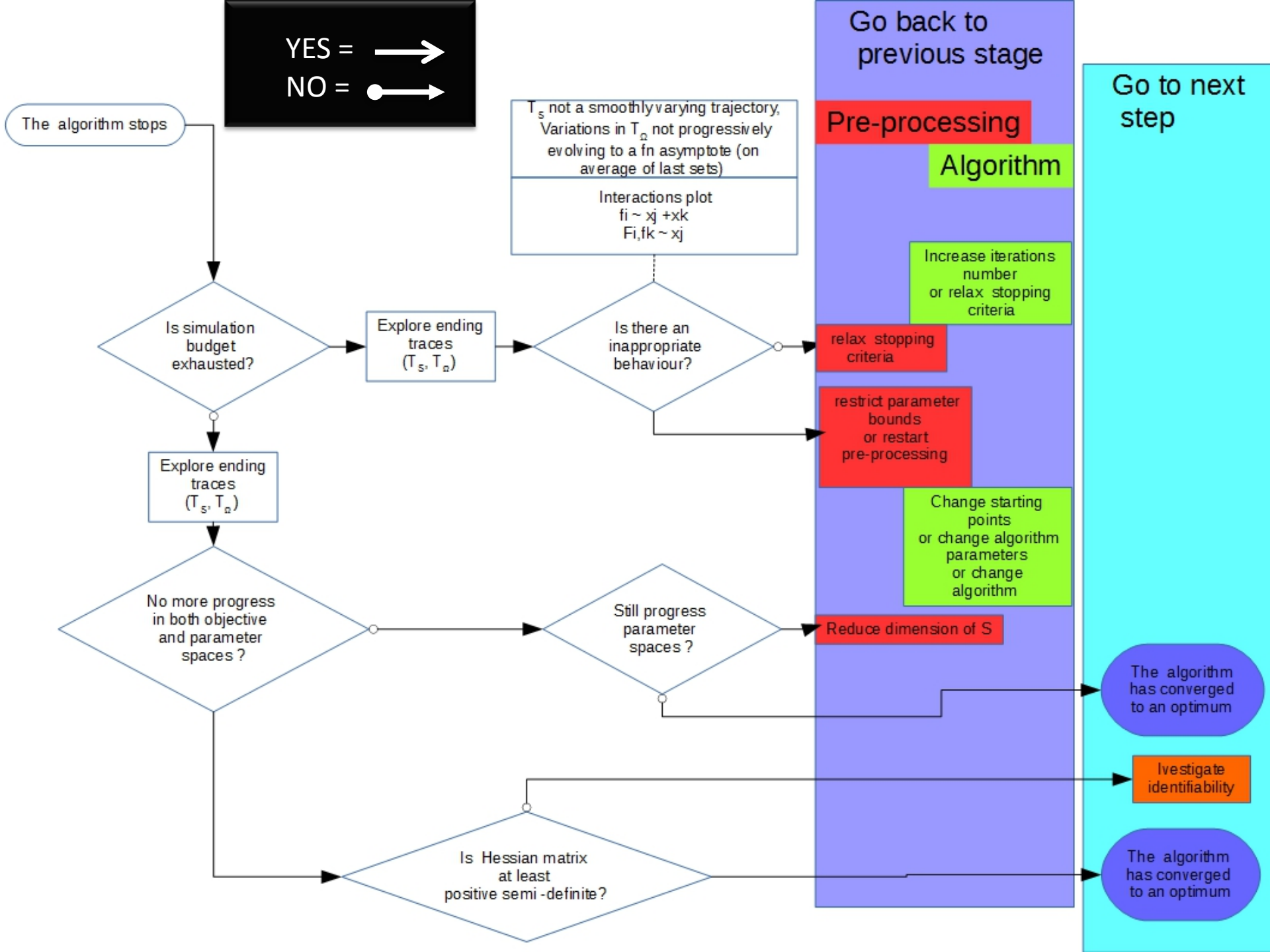


Espace paramètres

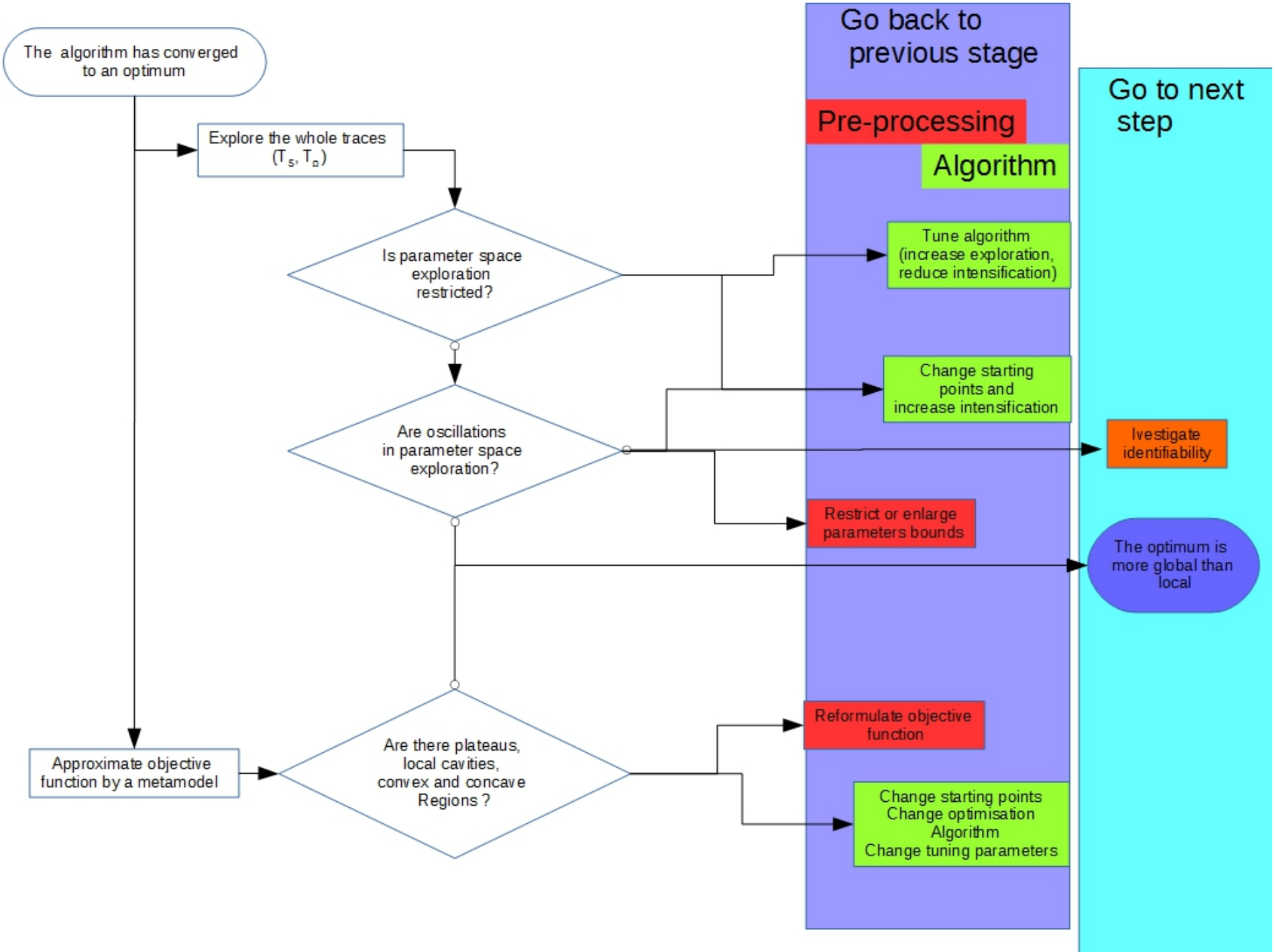


Hilaire Drouineau, TABASCO

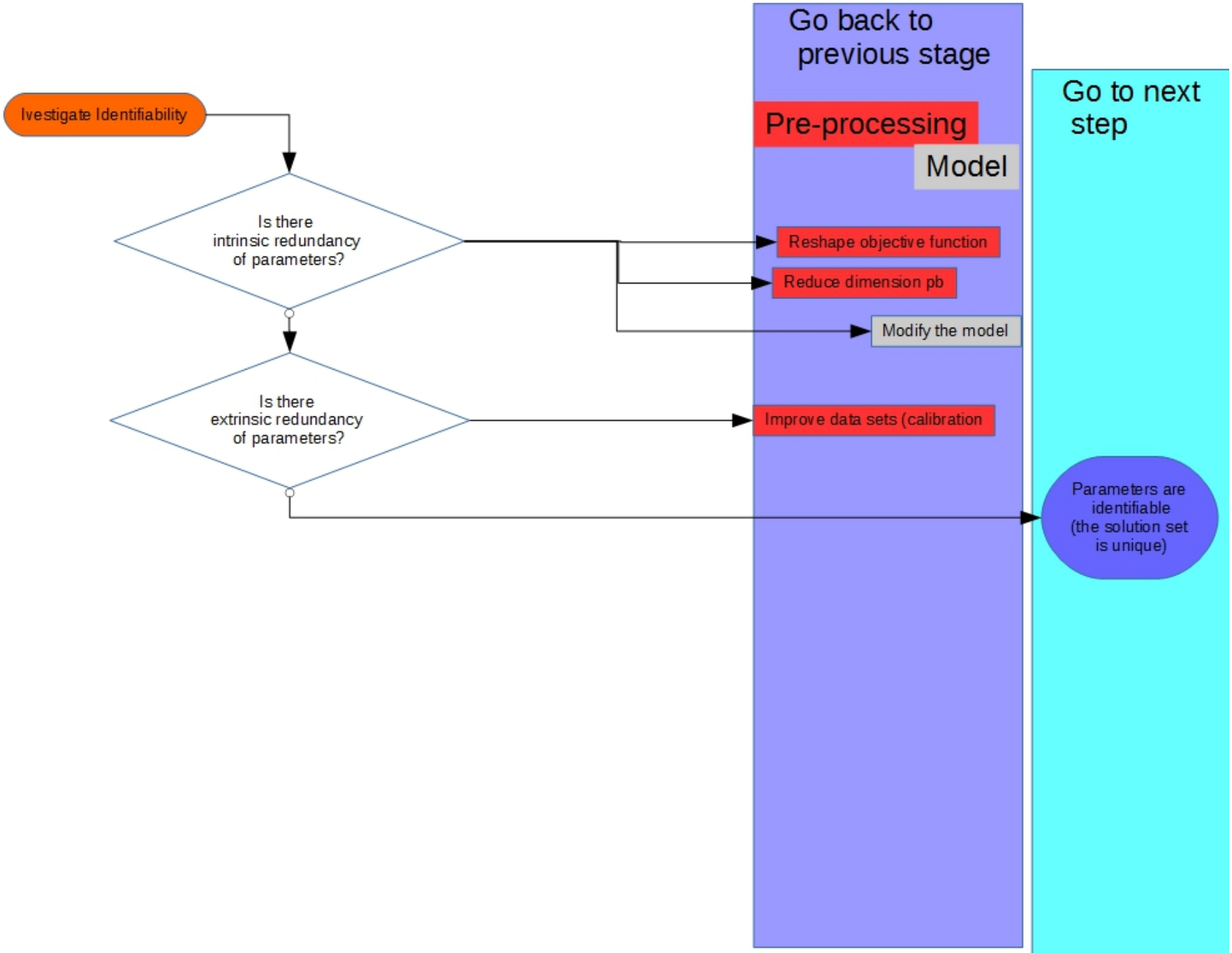
Convergence ?

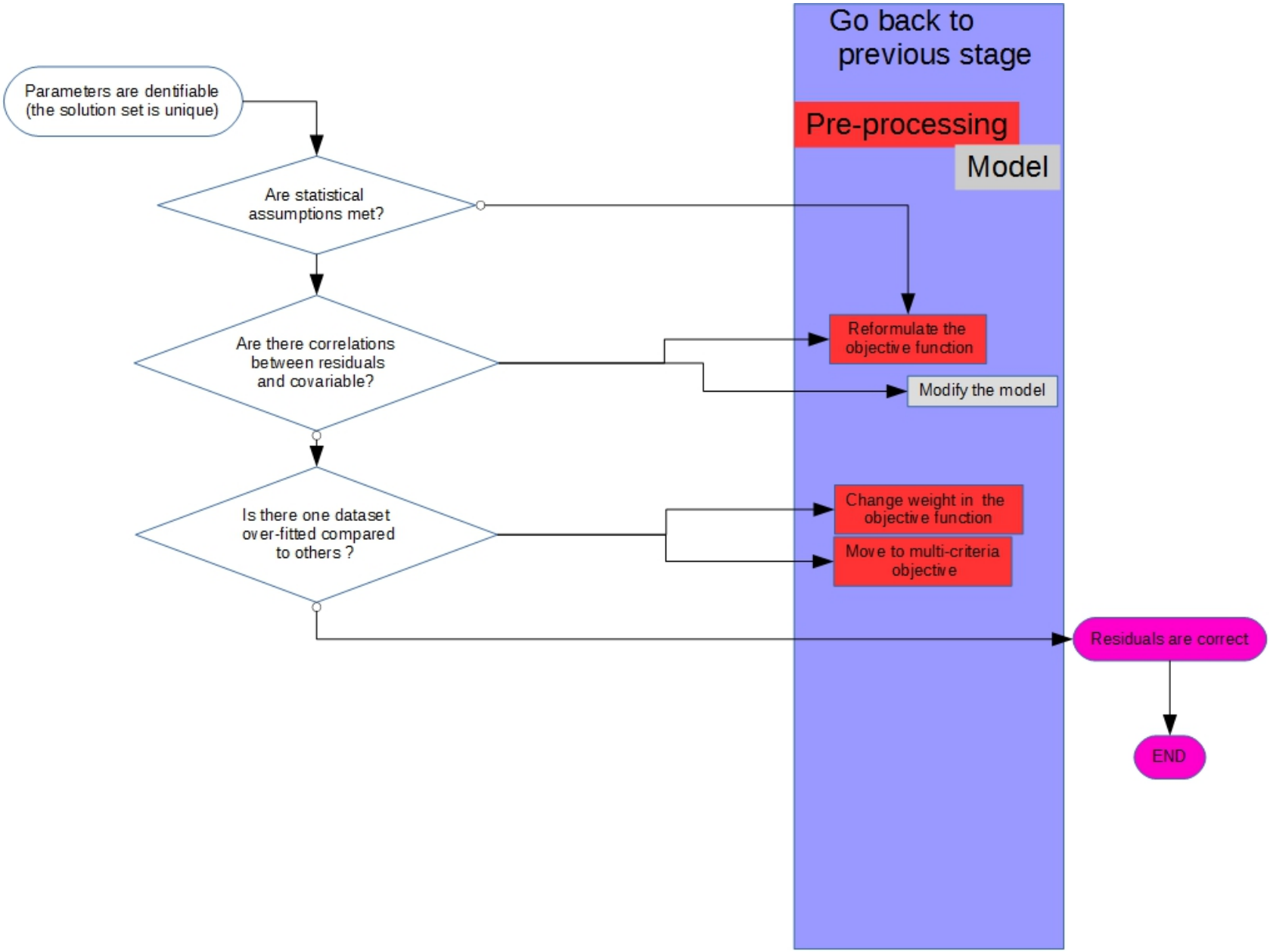

YES =
NO =
The algorithm stops
Is simulation budget exhausted?
Explore ending traces (T_s, T_Ω)
Is there an inappropriate behaviour?
T_s not a smoothly varying trajectory, Variations in T_Ω not progressively evolving to a fn asymptote (on average of last sets)
Interactions plot
fi ~ xj +xk
Fi,fk ~ xj
Go back to previous stage
Pre-processing
Algorithm
Go to next step
Increase iterations number or relax stopping criteria
relax stopping criteria
restrict parameter bounds or restart pre-processing
Change starting points or change algorithm parameters or change algorithm
Explore ending traces (T_s, T_Ω)
No more progress in both objective and parameter spaces ?
Still progress parameter spaces ?
Reduce dimension of S
The algorithm has converged to an optimum
Ivestigate identifiability
Is Hessian matrix at least positive semi -definite?
The algorithm has converged to an optimum

Qualité : Locale/globale?


The algorithm has converged to an optimum
Explore the whole traces (T_s, T_a)
Is parameter space exploration restricted?
Are oscillations in parameter space exploration?
Approximate objective function by a metamodel
Are there plateaus, local cavities, convex and concave Regions ?
Go back to previous stage
Pre-processing
Algorithm
Tune algorithm (increase exploration, reduce intensification)
Change starting points and increase intensification
Restrict or enlarge parameters bounds
Reformulate objective function
Change starting points
Change optimisation Algorithm
Change tuning parameters
Go to next step
Ivestigate identifiability
The optimum is more global than local

Qualité : identifiabilité ?


Go back to previous stage
Go to next step
Ivestigate Identifiability
Pre-processing
Model
Is there intrinsic redundancy of parameters?
Reshape objective function
Reduce dimension pb
Modify the model
Is there extrinsic redundancy of parameters?
Improve data sets (calibration
Parameters are identifiable (the solution set is unique)


Go back to previous stage
Pre-processing
Model
Parameters are dentifiable (the solution set is unique)
Are statistical assumptions met?
Are there correlations between residuals and covariable?
Is there one dataset over-fitted compared to others ?
Reformulate the objective function
Modify the model
Change weight in the objective function
Move to multi-criteria objective
Residuals are correct
END

Traçabilité, Reproductibilité et Archivage

ODDOdo : Overview Description and Details of Optimization

dans la continuite du ODD de Grimm *et al,* 2010

Model	Performance	Time per model run	
		parallelisation	
	Development	language	
		Implementation of the optimisation algorithm	

Pre-processing	Problem Formulation	Model	
		Question	
		Data	
		Parameters Bounds&constrainsts	
		Uncertainty (process and data)	
		Initial objective function	
	Objective Function	building	
		reshaping	
		final	
	Exploratory Analysis	data	
		Reduction dimension	

Algorithm	Family	
	Description-Justification	
	Changes in the algorithm	
	Settings	

Post-processing	Convergence	
	Optimum properties including Identifiability	
	Residual analysis	
	Multicriteria	

Comment	Number of simulations required
	Duration
	Reached stopping criteria

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