An introduction to calibration of complex models illustrated with fisheries models

Stéphanie Mahévas

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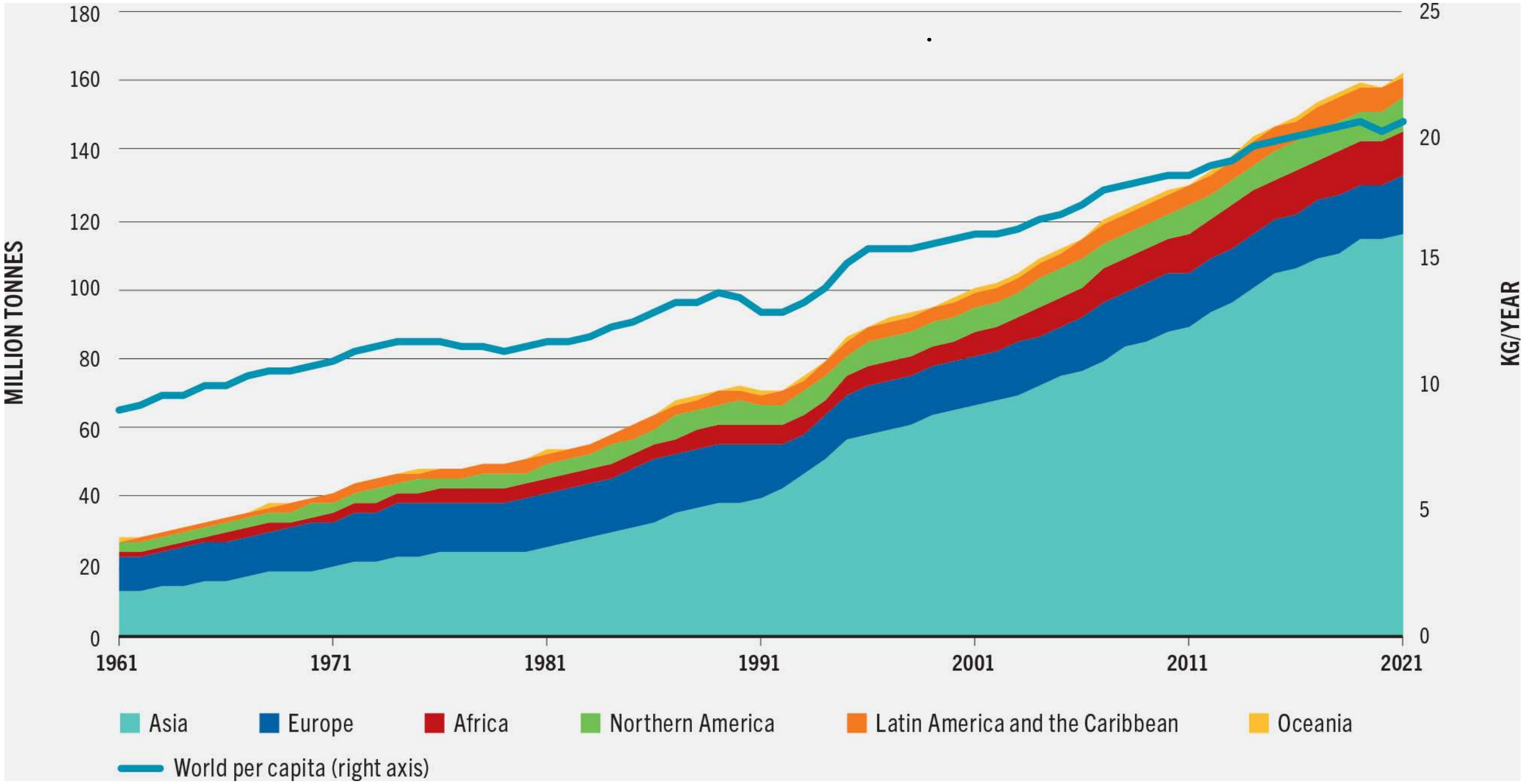
Univ Montpellier, IRD, CNRS, IFREMER, Sète

TED4LAT workshop and doctoral school - 21-25 October 2024 - Paris

Context of fisheries and fisheries modelling

APPARENT CONSUMPTION OF AQUATIC ANIMAL FOODS BY REGION, 1961–2021

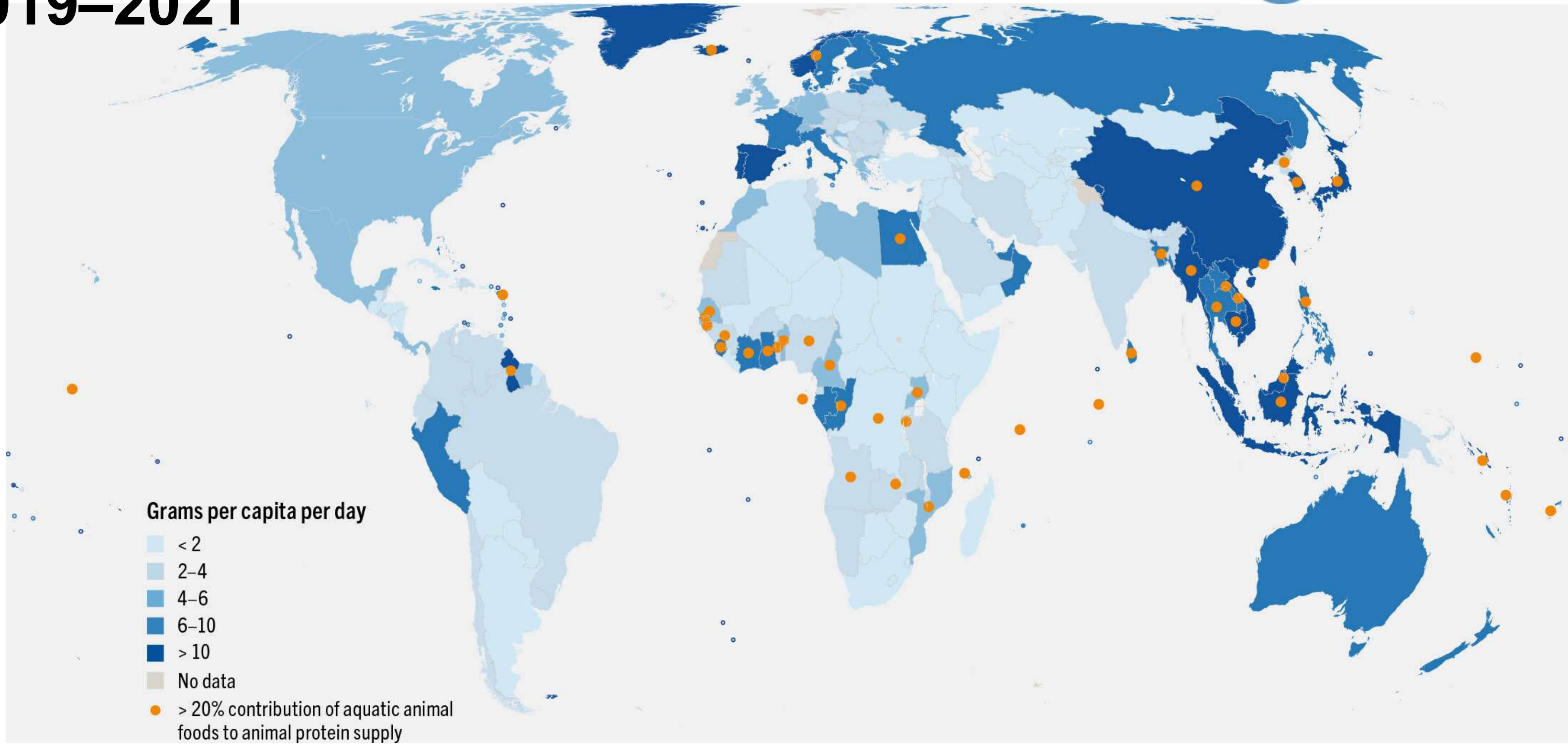


FAO. 2024. *The State of World Fisheries and Aquaculture 2024 – Blue Transformation in action.* Rome.

Food and Agriculture Organization of the United Nations

- We eat more and more aquatic food.
- For sixty years, the global amount of aquatic animal foods available for human consumption has increased at a significantly higher rate (3%) than world population growth (1.6%)

CONTRIBUTION OF AQUATIC ANIMAL FOODS TO ANIMAL PROTEIN SUPPLY PER CAPITA, AVERAGE 2019–2021

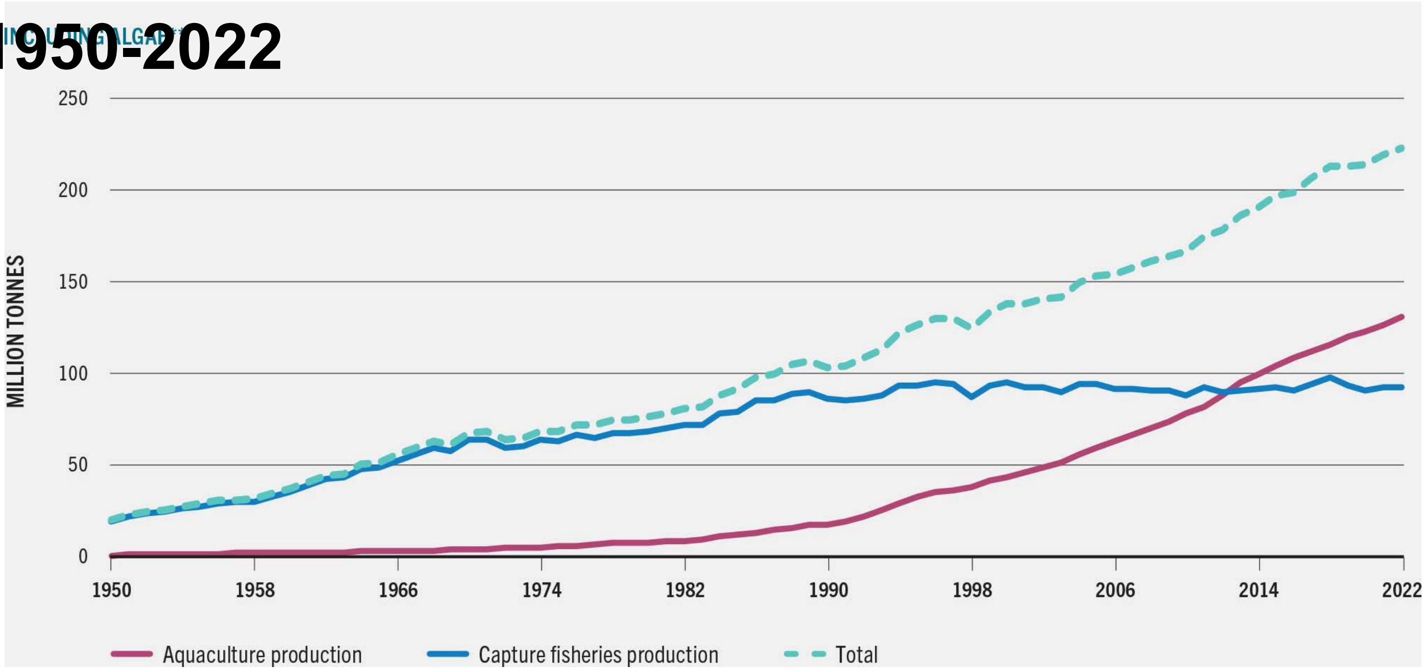


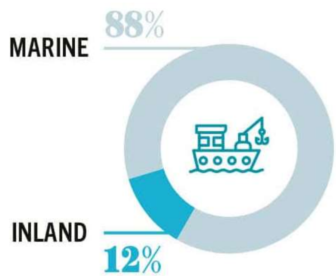
FAO. 2024. *The State of World Fisheries and Aquaculture 2024 – Blue Transformation in action*. Rome.

- Globally, aquatic animal foods supplied 15 % of animal proteins and 6 % of all proteins in 2021.

- The extent of their contribution varies from country to country : 14 % in low-income countries, 18 % in lower-middle-income countries, 17 % in upper-middle-income countries, and 10 % in high-income countries.

WORLD FISHERIES AND AQUACULTURE PRODUCTION
1950-2022



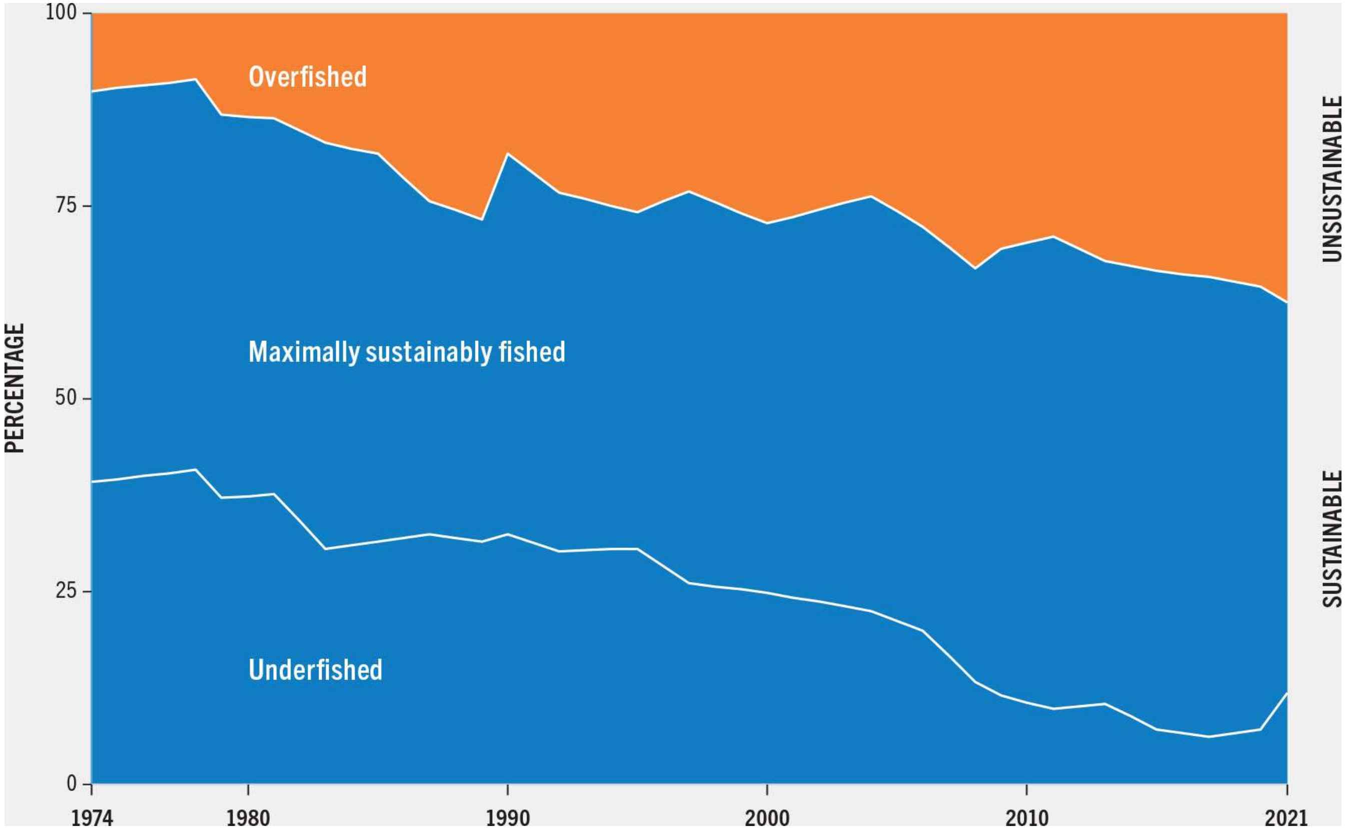


FAO. 2024. *The State of World Fisheries and Aquaculture 2024 – Blue Transformation in action*. Rome.

- Global fisheries catches have been relatively stable since the late 1980s, and remain below 100 million tonnes and in 2022 88% catches are from the sea

- On the other hand during the same period, aquaculture has grown significantly , exceeding fisheries catches in 2012 and 100 million tonnes in 2014

GLOBAL TRENDS IN THE STATE OF THE WORLD'S MARINE FISHERY STOCKS, 1974–2021



Food and Agriculture Organization of the United Nations

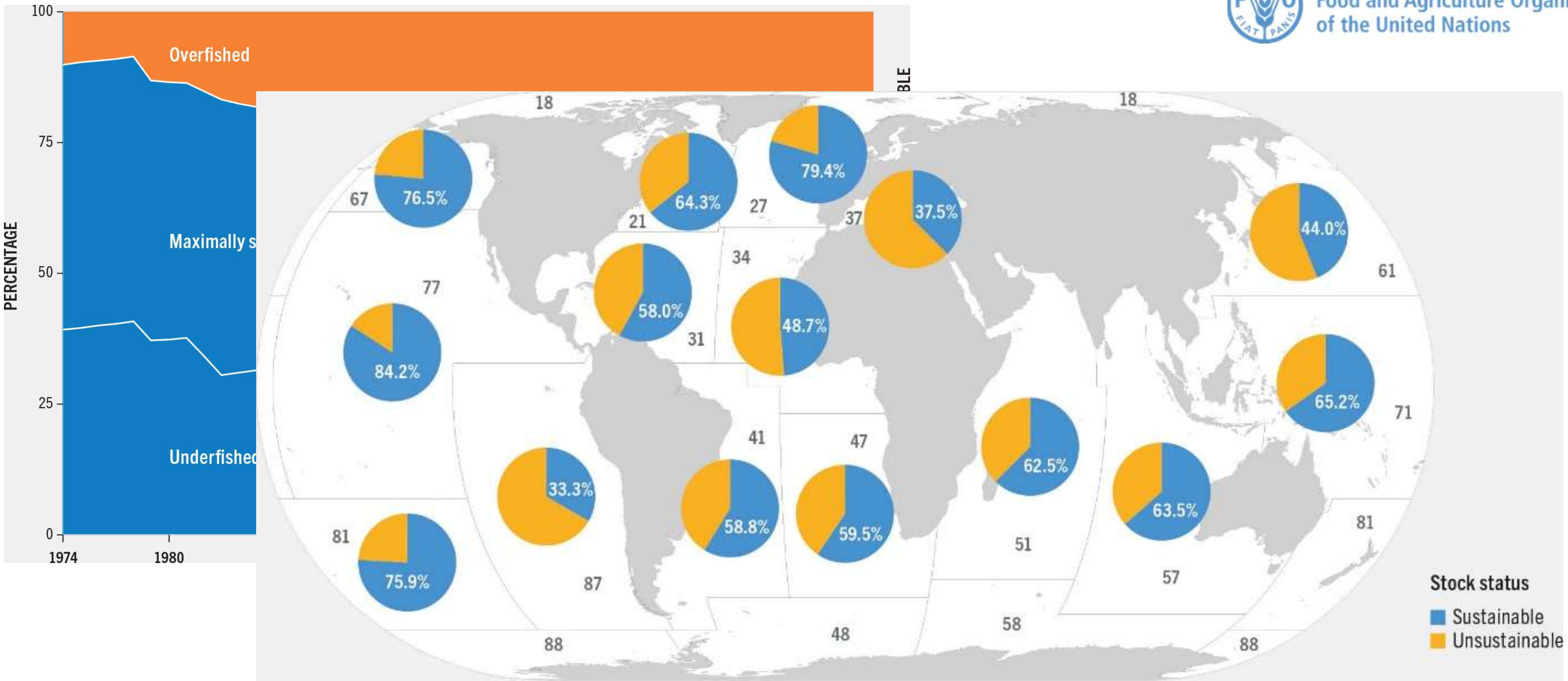
FAO. 2024. *The State of World Fisheries and Aquaculture 2024 – Blue Transformation in action*. Rome.

- In 2011, biologically sustainable stocks (maximally sustainably fished and underfished) account for 62,3 % of the total number of assessed stocks

- The % of overfished stocks still increased at the world level

GLOBAL TRENDS IN THE STATE OF THE WORLD’S MARINE FISHERY STOCKS, 1974–2021

Food and Agriculture Organization of the United Nations



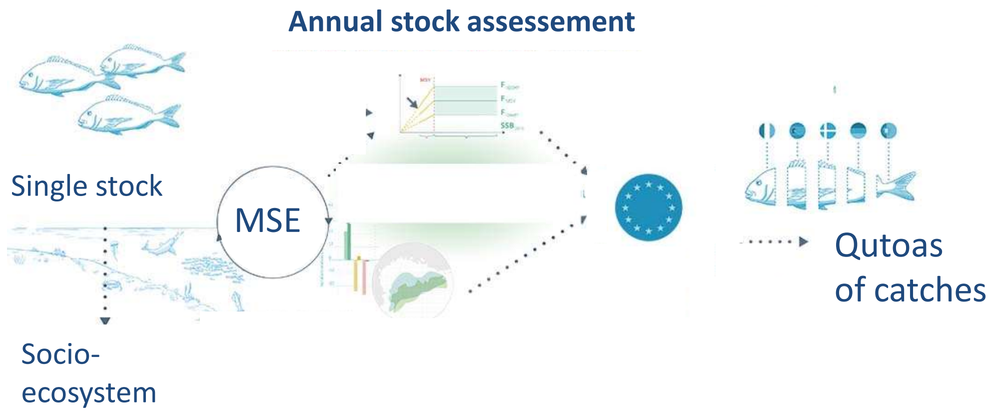
FAO. 2024. *The State of World Fisheries and Aquaculture 2024 – Blue Transformation in action*. Rome.

- The % of overfished stocks still increased at the world level
- Differences in proportion region by region and in trend with for instance slightly decrease trend of overfished stocks in Northeast Atlantic

Managing fishing is therefore a global challenge

- to conserve Marine Biodiversity (human fishing activity is one of the most direct and effective impacting pressure on marine biodiversity) and
- to provide marine proteins to human in a sustainable way

The ecosystem based approach of fisheries management

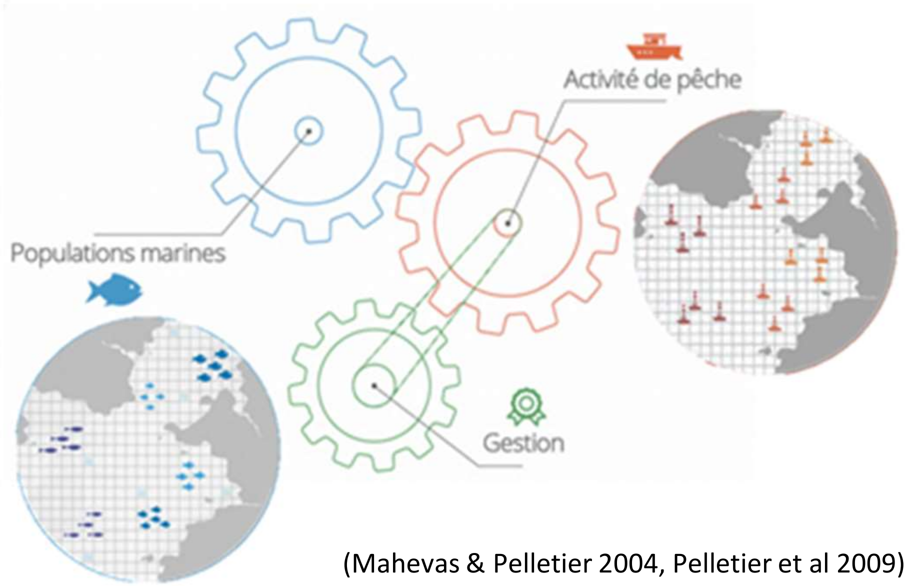


Mahévas et al In prep

In the north of Europe, fisheries management is mainly dominated by quotas management measures that are supported on one hand by annual stock assessment stock by stock and on second hand by socio-ecosystem approach through Multi-annual Management Plan

The ecosystem based approach of fisheries management

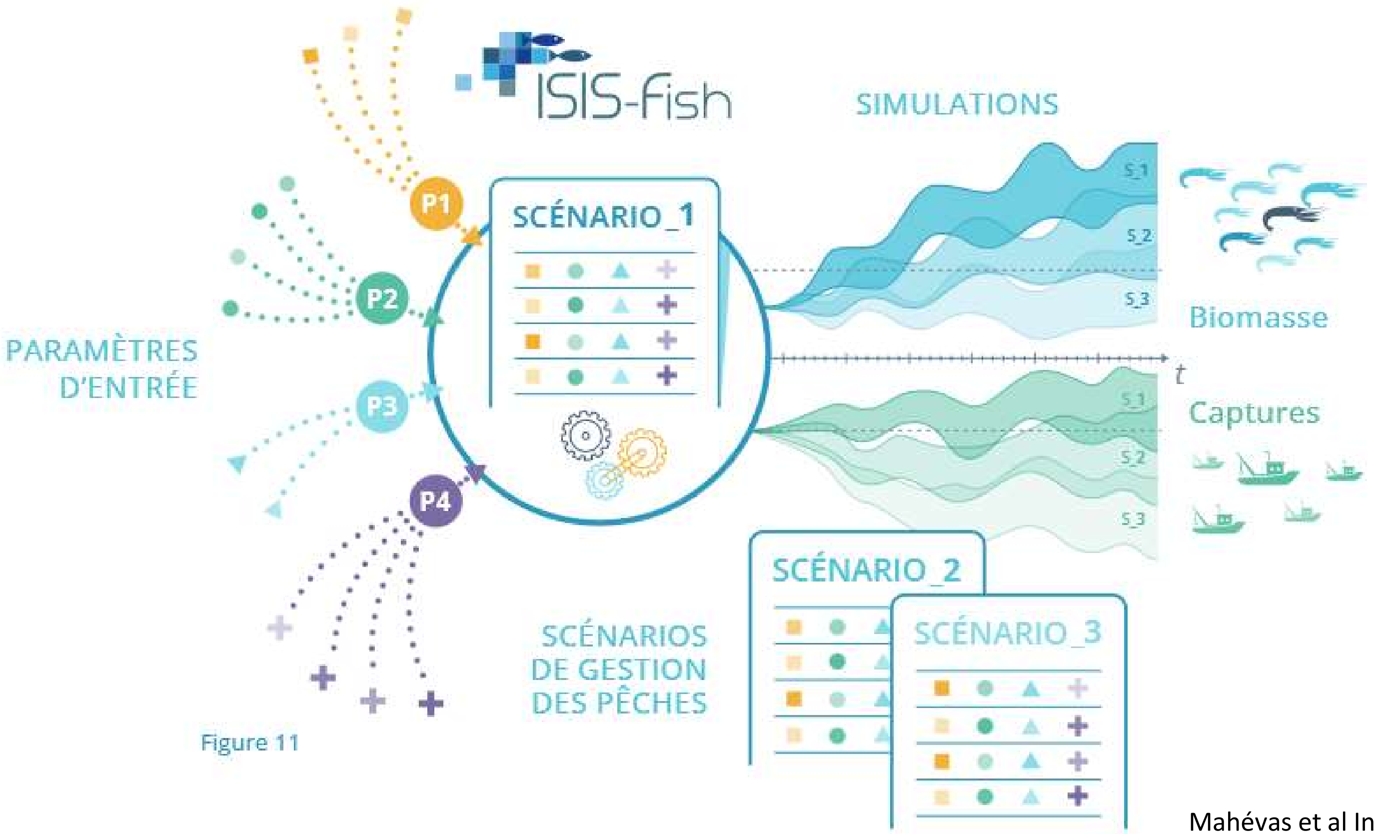
In both approaches simple and complex Models are usual and necessary tools for providing management advice uncluding uncertainty analysis that are link to the multiple uncertainties in the knowledge of fisheries functioning.



(Mahevas & Pelletier 2004, Pelletier et al 2009)

ISIS-Fish model describes the spatial an monthly dynamics of fisheries including
1) a management module to define fishing regulations
2) a fishing activities module to parametrize the fishing vessels dynamics
3) a population module to parametrize the fish life cycle

Short movie on https://isis-fish.org



Mahévas et al In prep

Once the model has been parameterized, management scenarios can be simulated accounting for uncertainty and the consequences on vessels catches and fish biomass can be analyzed to provide advice on fishing regulations (quotas, Marine Protected Area, …)

- a national research network involving reaserchers from INRAE, IFREMER, CIRAD, University…
- Animation and development of practical methods for exploring complex models like ISIS-fish. These methods include sensitivity analysis, calibration, …
- https://reseau-mexico.fr

mexico2024 : Rencontres annuelles 2024 du réseau Mexico

5-6 déc. 2024 Villeurbanne (France)

https://reseau-mexico.fr

mexico2024 : Rencontres annuelles 2024 du réseau Mexico

5-6 déc. 2024 Villeurbanne (France)

A Practical Guide for Conducting Calibration and Decision-Making Optimisation with Complex Ecological Models (2019)

Mahévas, S.; Picheny, V.; Lambert, P.; Dumoulin, N.; Rouan, L.; Soulié, J.-C.; Brockhoff, D.; Lehuta, S.; Le Riche, R.; Faivre, R.; Drouineau, H.

Preprints 2019120249. https://doi.org/10.20944/preprints201912.0249.v1

Calibration

- Calibration : what is calibration?
- Why calibrate a model?
- How calibrating a complex model?

- Calibration : what is calibration?

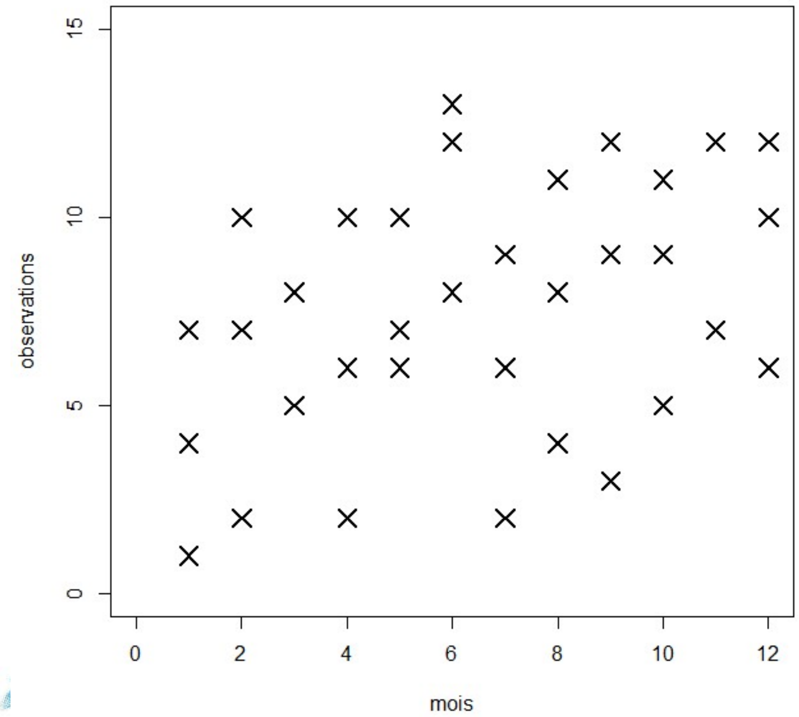
Calibration : what is calibration ?

- In metrology: comparison with a test device that faithfully reflects the standard measurement.
- In statistics: method of estimating (inverse method) parameters - given x and y=f(x), knowing y, we look for x (=f^-1(y))
- Model calibration: process of adjusting the parameters of a model by integrating the uncertainty of the parameters and/or of the model to obtain a representation of the modeled system that satisfies a predefined criterion

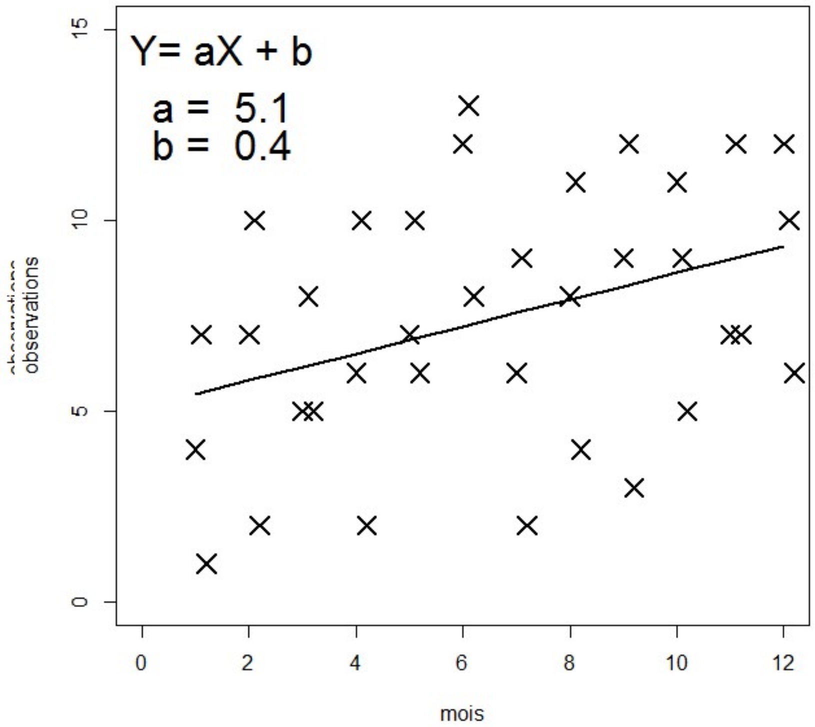
Data assimilation is a form of calibration (weather or physical model, …)

Calibration of linear model (2 parameters)

Set of monthly observations



What is the best 2-parameter linear model to reproduce this set of observations?



Y = 5.1 + 0.35 month

Complex model

- 2-parameter linear model: analytical resolution - least-squares estimation
- Complex models
  - Numerous parameters
  - Numerous outputs
  - Poorly understood processes

The problem gets more complicated

- Why calibrate a model?

Why calibrate a model?

- Estimate parameters that are difficult or impossible to measure
- Understand the workings of the system under study (when several hypotheses coexist)
- Give credibility to/improve a model for use in decision-making, prediction, etc.

Contents lists available at ScienceDirect
ELSEVIER
Environmental Modelling & Software
journal homepage: www.elsevier.com/locate/envsoft

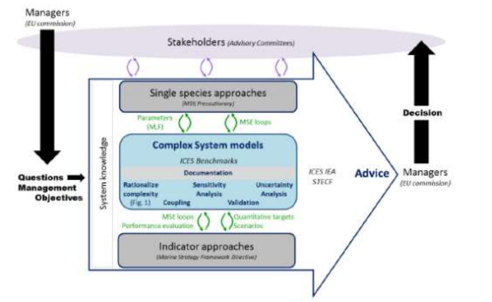
Optimisation as a process for understanding and managing river ecosystems

E.J. Barbour [a, b, *], L. Holz [c], G. Kuczera [d], C.A. Pollino [e], A.J. Jakeman [a], D.P. Loucks [f]

Contents lists available at SciVerse ScienceDirect
ELSEVIER
Fisheries Research
journal homepage: www.elsevier.com/locate/fishres

Selection and validation of a complex fishery model using an uncertainty hierarchy

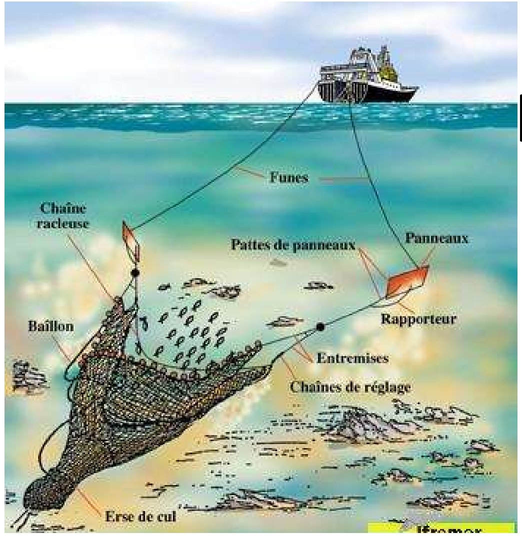
Sigrid Lehuta [a,*], Pierre Petitgas [a], Stéphanie Mahévas [a], Martin Huret [b], Youen Vermard [c], Andrés Uriarte [d], Nicholas R. Record [e]



Reconciling complex system models and fisheries advice: Practical examples and leads

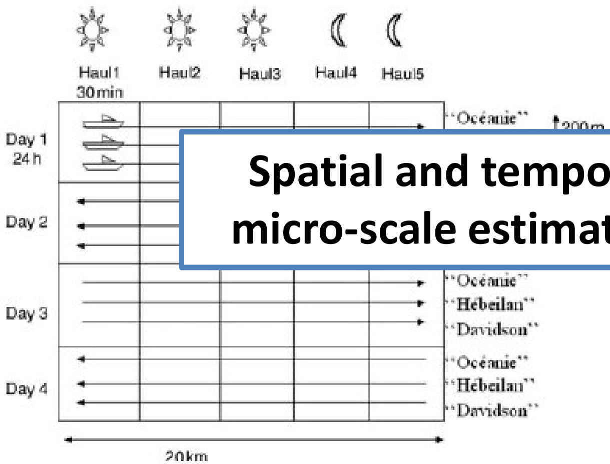
Sigrid LEHUTA[1,a], Raphaël GIRARDIN[2], Stéphanie MAHÉVAS[1], Morgane TRAVERS-TROLET[2] and Youen VERMARD[1]

Hard-to-measure parameters

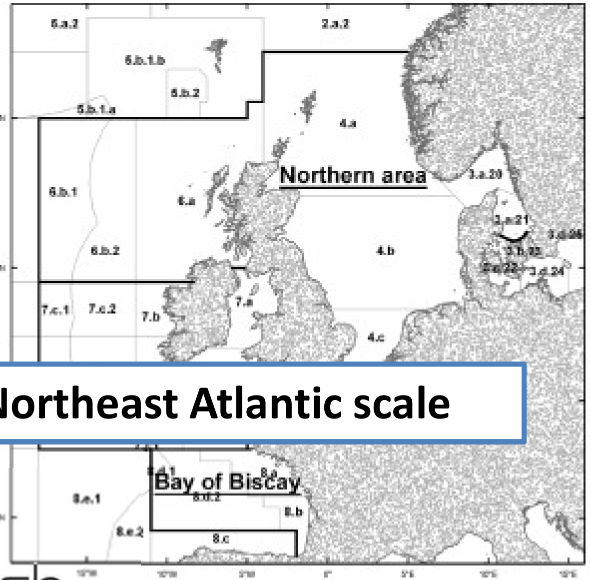


Hake *(merluccius merluccius)* catchability **q**

Catch~=**q** x Effort x Abundance



Spatial and temporal micro-scale estimation



Northeast Atlantic scale

ISIS-Fish

Saison	1	2	3	4
Valeur $q_s = q_s^0$	$1.69 * 10^{-6}$	$8.20 * 10^{-7}$	$7.24 * 10^{-7}$	$7.63 * 10^{-7}$

ICES Journal of Marine Science (2011), 68(1), 107–118. doi:10.1093/icesjms/fsq140

Hake catchability by the French trawler fleet in the Bay of Biscay: estimating technical and biological components

Stéphanie Mahévas*, Verena M. Trenkel, Mathieu Doray, and Arnaud Peyronnet

marbec

scientific data

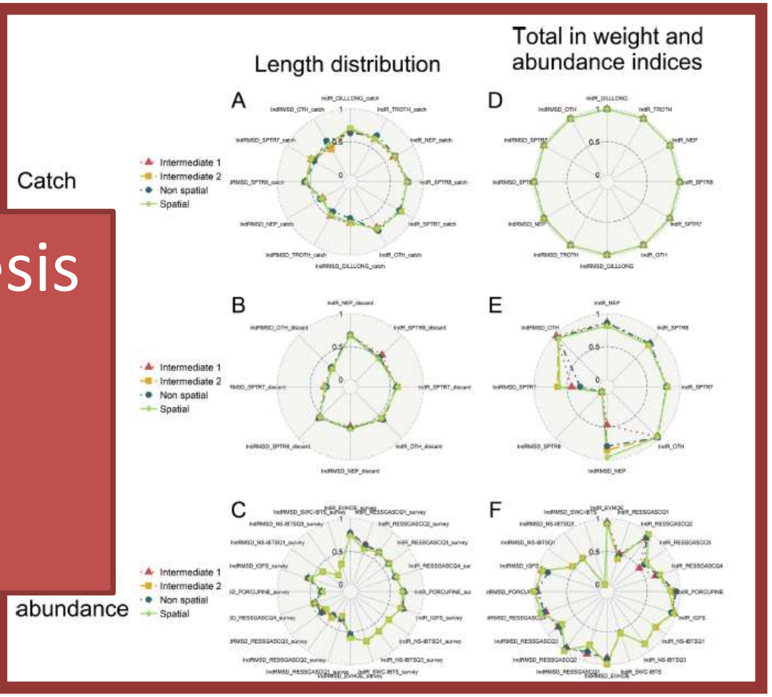
OPEN
DATA DESCRIPTOR

Monthly spatial dynamics of the Bay of Biscay hake-sole-Norway lobster fishery: an ISIS-Fish database

Audric Vigier, Michel Bertignac & Stéphanie Mahévas

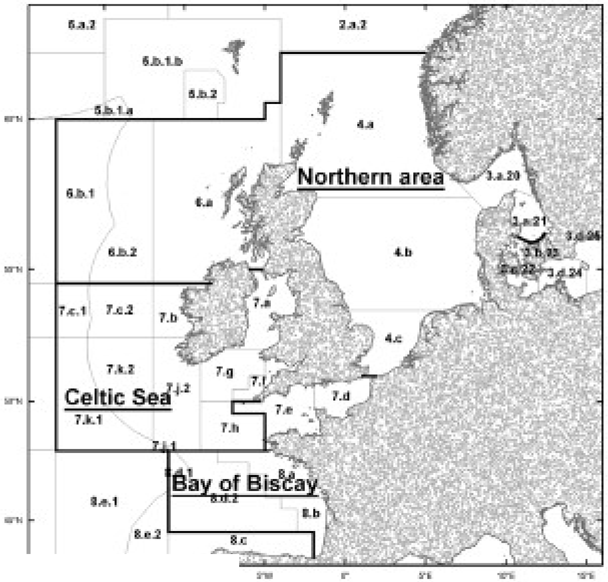
Understanding the system

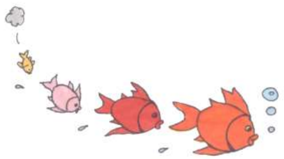
Spatial and temporal dynamics of the hake population in the Northeast Atlantic



Stock Synthesis

likelihood





Fisheries Research 199 (2018) 158–170

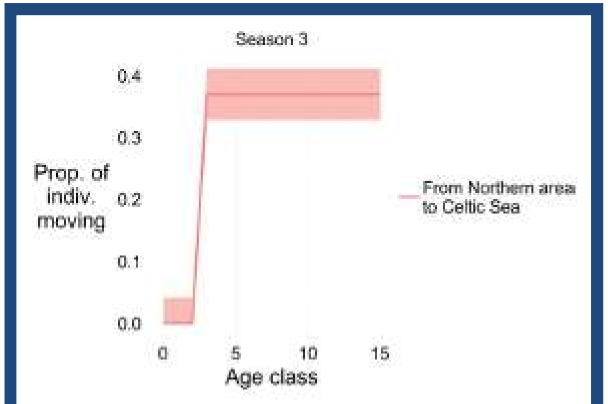
Contents lists available at ScienceDirect

Fisheries Research

journal homepage: www.elsevier.com/locate/fishres

Towards a spatial integrated stock assessment model for European hake northern stock

Audric Vigier[a,b,*], Stéphanie Mahévas[a], Michel Bertignac[b]



Improving the accuracy of model outputs

BEFORE CALIBRATION

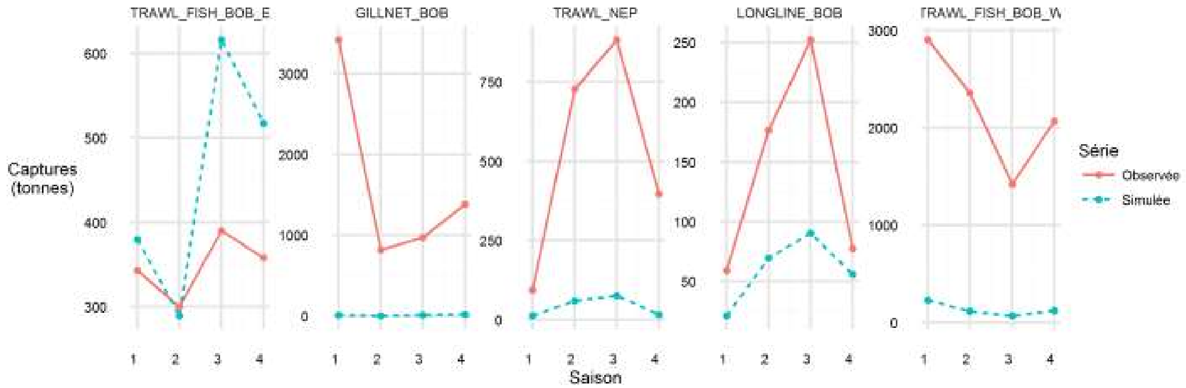


FIGURE 3.5 – Ajustement des captures simulées par ISIS-Fish (trait pointillé) aux captures observées (trait plein) pour 2010 par super-métier (cadran) et saison (abscisse) à l'étape 1 pour $q^p = 0.85$.

AFTER CALIBRATION

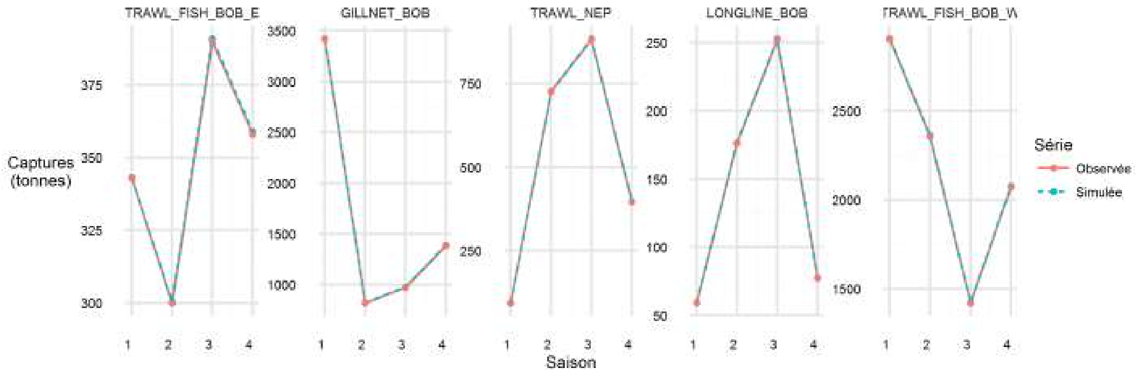
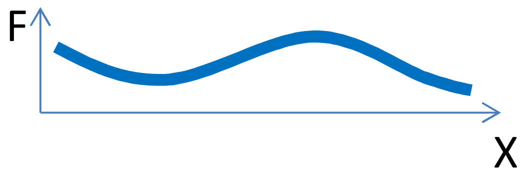


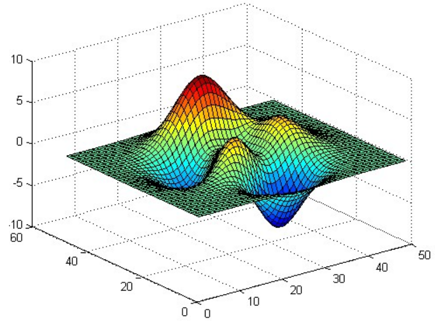
FIGURE 3.7 – Ajustement des captures simulées par ISIS-Fish (trait pointillé) aux captures observées (trait plein) pour 2010 par super-métier (cadran) et saison (abscisse) à l'itération 3 de l'étape 2 pour $Tarf^p = 1$.

Vigier, A., Bertignac M., Mahévas S. 2022

Why is it so difficult to calibrate complex models?

- **Number of parameters: very large exploration space** **(space dimension = number of parameters)**





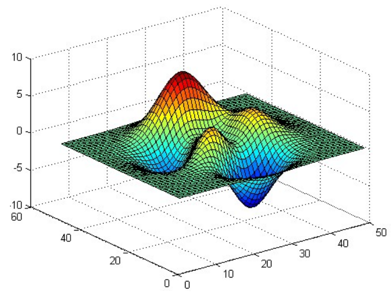
• • •

1 parameter   2 parameters   Many parameters

- **Simulation time: costly evaluation for one parameter value**

several minutes   to   several hours

- **Multi-modalities**



- **Stochasticity**

- How calibrating a complex model ?

Calibration

parameters
X

Model
M(X)

Outputs
Y*sim*

Observations
Y*obs*

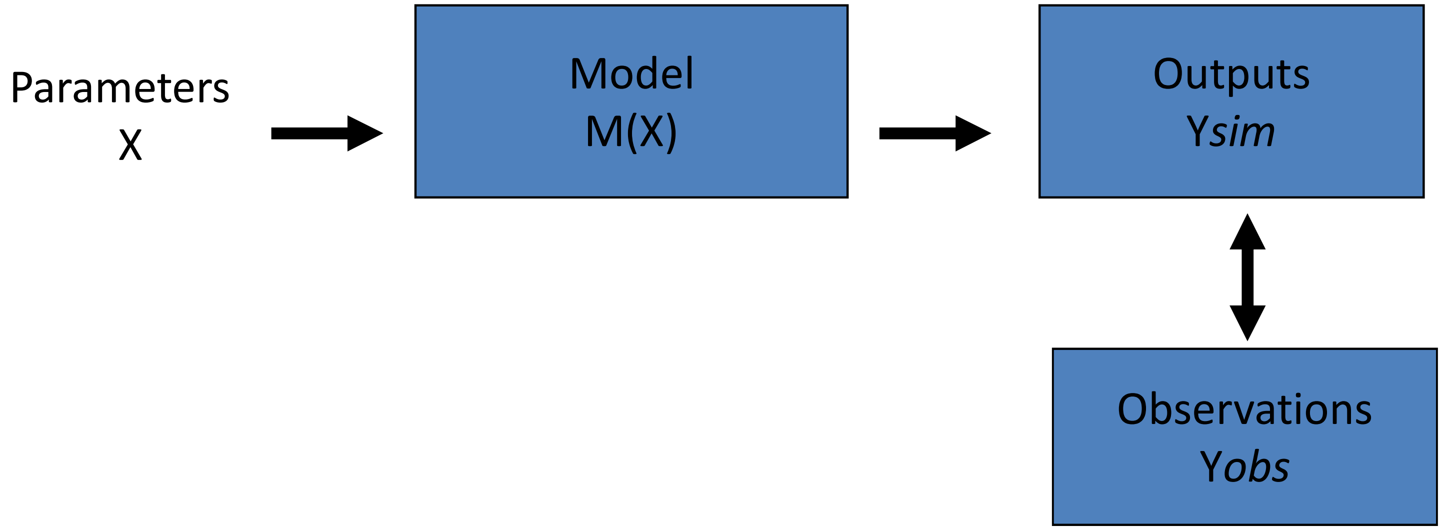
F(X) = dist(Y*sim*,Y*obs*) = dist(M(X),Y*obs*)

X?
Xopt= Arg(min(dist(Y*sim*,Y*obs*))

Non-analytical F
Non-linear, multimodal,...
Costly to evaluate

Optimization - numerical approach
Optimizer = iterative algorithm

Calibration



X?

***Xopt*= Arg(min(dist(*Ysim*,*Yobs*))**)

X_i^1: $M(X_i^1) = Ysim^1$ → X_i^2: $M(X_i^2) = Ysim^2$ … → X_i^n: $M(X_i^n) = Ysim^n$

Yobs → F^1 → X_i^2

Yobs → F^2 → X_i^2

Yobs → $F^n < \varepsilon$

$X_i = X_i^n$

CALIBRATION

=

Optimizing a mathematical function

No distribution assumption on **Y**
No distribution assumption on **X**

Distribution assumption on **Y**
No distribution assumption on **X**

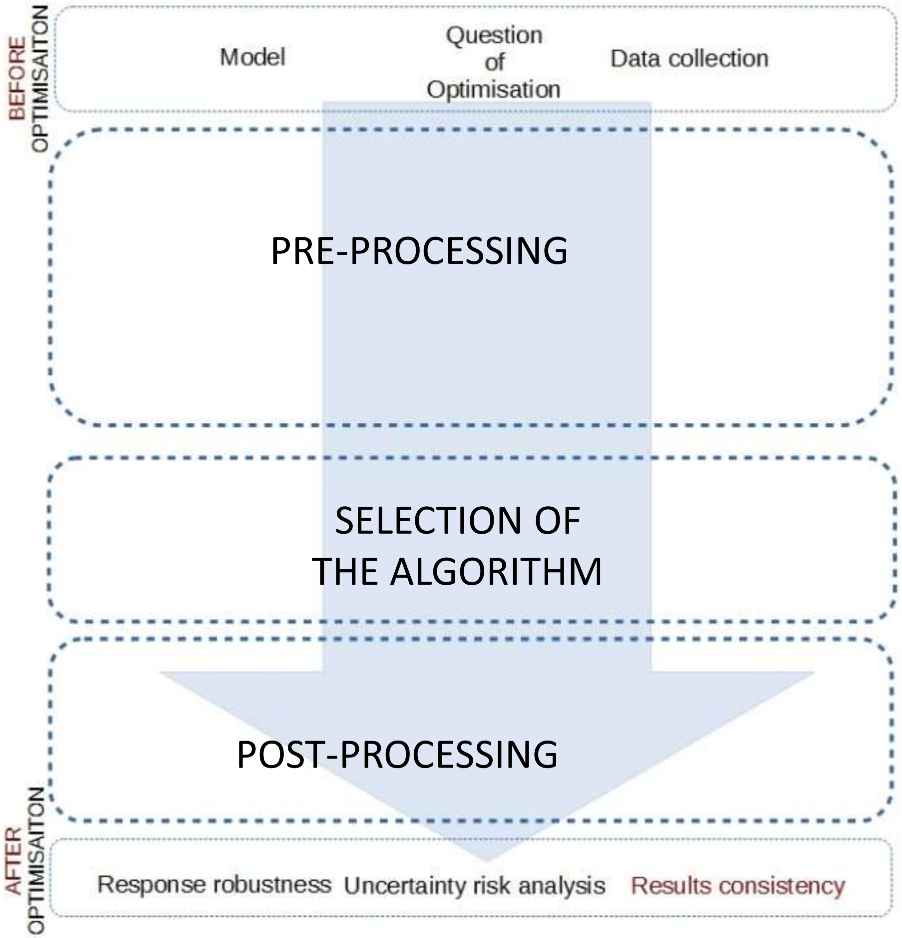
Distribution assumption on **Y**
Distribution assumption on **X**

Numerical analysis

Inferential statistics

Bayesian statistics

Calibration implementation



Pre-processing : F and Ω_X

Seldom… if ever explained

Essential classics :

- Clarifying the optimization issue
  Predictive capacity of the model? Parameter values? System understanding?
- List of available data: observations, expert knowledge
- List of all parameters to be estimated: limits, constraints, discrete/continuous
- List uncertainties: data, process (model)

Pre-processing: : F and Ω_X

Seldom… if ever explained

Essential classics :

- Clarifying the optimization issue
- List of available data:
- List of all parameters to be estimated:
- List uncertainties:
- Build an initial objective function: most critical point

F(X) = dist(Y*sim*,Y*obs*) = dist(M(X),Y*obs*)

The most common: least squares, likelihood

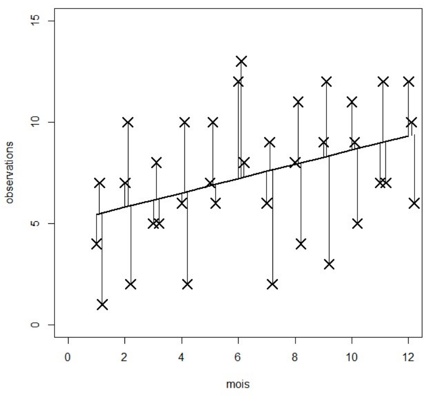
Most specific: statistics for approximate Bayesian computation (ABC) (Fearnhead and Prangle, 2012)

Multi-objective: weights (Francis, 2011),

Pareto fronts (dominance, >4 difficulty) (Deb and Sundar, 2006)

$$F(X) = \sum_{k=0}^{n} (M(X) - Yobs)^2$$

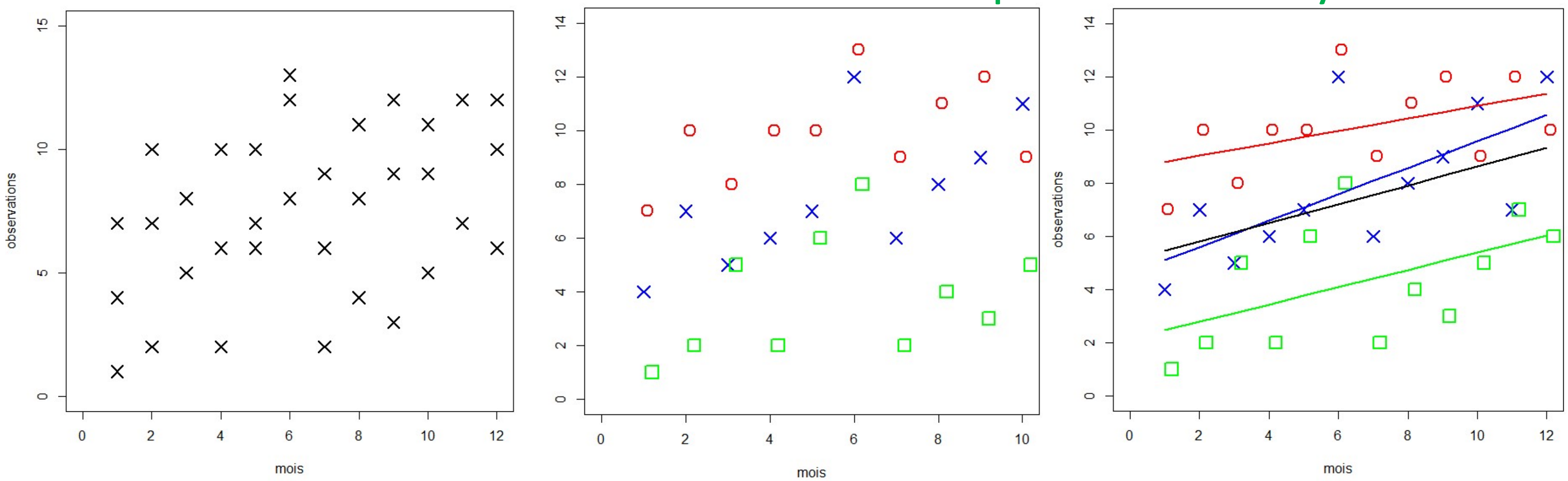
$$F(X) = L(Y = Yobs|X)$$



Set of monthly observations

Spatial heterogeneity

Temporal variability



O Area 1- Year 1 X Area 2 – Year 1 □ Area 1- Year 2

M(X) → M’(X’)

F(X’) = αF1(X’) + βF2(X’) + γF3(X’)

$$FO = \sum_{\substack{p\in P\\ s\in S\\ Smet\in SMET}} (\omega^{LFD}_{Smet,p,s} * \alpha * FO_1 + \omega^{weight}_{Smet,p,s} * (\beta * FO_2 + \gamma * FO_3))$$

$$FO_1 = \left(\frac{C^{obs}_{Smet,l,s,p}}{\sum_{l\in L} C^{obs}_{Smet,l,s,p}} - \frac{C^{sim}_{Smet,l,s,p}}{\sum_{l\in L} C^{sim}_{Smet,l,s,p}}\right)^2$$

$$FO_2 = \left(\frac{\sum_{l\in L} C^{obs}_{Smet,l,s,p} - \sum_{l\in L} C^{sim}_{Smet,l,s,p}}{\sum_{l\in L} C^{obs}_{Smet,l,s,p}}\right)^2$$

$$FO_3 = \left(\frac{\sum_{\substack{l\in L\\ s\in year}} C^{obs}_{Smet,l,s,p} - \sum_{\substack{l\in L\\ s\in year}} C^{sim}_{Smet,l,s,p}}{\sum_{\substack{l\in L,\\ s\in year}} C^{obs}_{Smet,l,s,p}}\right)^2$$

ISIS-Fish

Ifremer

marbec

MEXICO

Pre-processing

Seldom... if ever explained

Essential classics :

- Clarifying the optimization issue
- List of available data
- List of all parameters to be estimated
- List uncertainties
- Build an initial objective function

Less classic essentials:

- Data mining and dimension reduction

  outliers, overdispersion, correlations, etc. and sensitivity analysis, PCA,...

- Objective function exploration and adaptation

  re-parametrization, which involves transforming the objective function and/or variables (Bolker et al 2013)

Which algorithm?

Abundant literature (highly technical, especially for computer scientists)

J Glob Optim (2013) 56:1247–1293
DOI 10.1007/s10898-012-9951-y

Derivative-free optimization: a review of algorithms and comparison of software implementations

Luis Miguel Rios · Nikolaos V. Sahinidis

Struct Multidisc Optim (2010) 41:219–241
DOI 10.1007/s00158-009-0420-2

RESEARCH PAPER

Survey of modeling and optimization strategies to solve high-dimensional design problems with computationally-expensive black-box functions

Songqing Shan · G. Gary Wang

J Glob Optim (2009) 45:3–38
DOI 10.1007/s10898-008-9332-8

A review of recent advances in global optimization

C. A. Floudas · C. E. Gounaris

HYDROLOGICAL PROCESSES
Hydrol. Process. (2008)
Published online in Wiley InterScience
(www.interscience.wiley.com) DOI: 10.1002/hyp.7152

Evaluation of global optimization algorithms for parameter calibration of a computationally intensive hydrologic model

Xuesong Zhang,[1,2]* Raghavan Srinivasan,[1] Kaiguang Zhao[1] and Mike Van Liew[3]

Environmental Modelling & Software 34 (2012) 67–86
Contents lists available at SciVerse ScienceDirect
Environmental Modelling & Software
journal homepage: www.elsevier.com/locate/envsoft
ELSEVIER

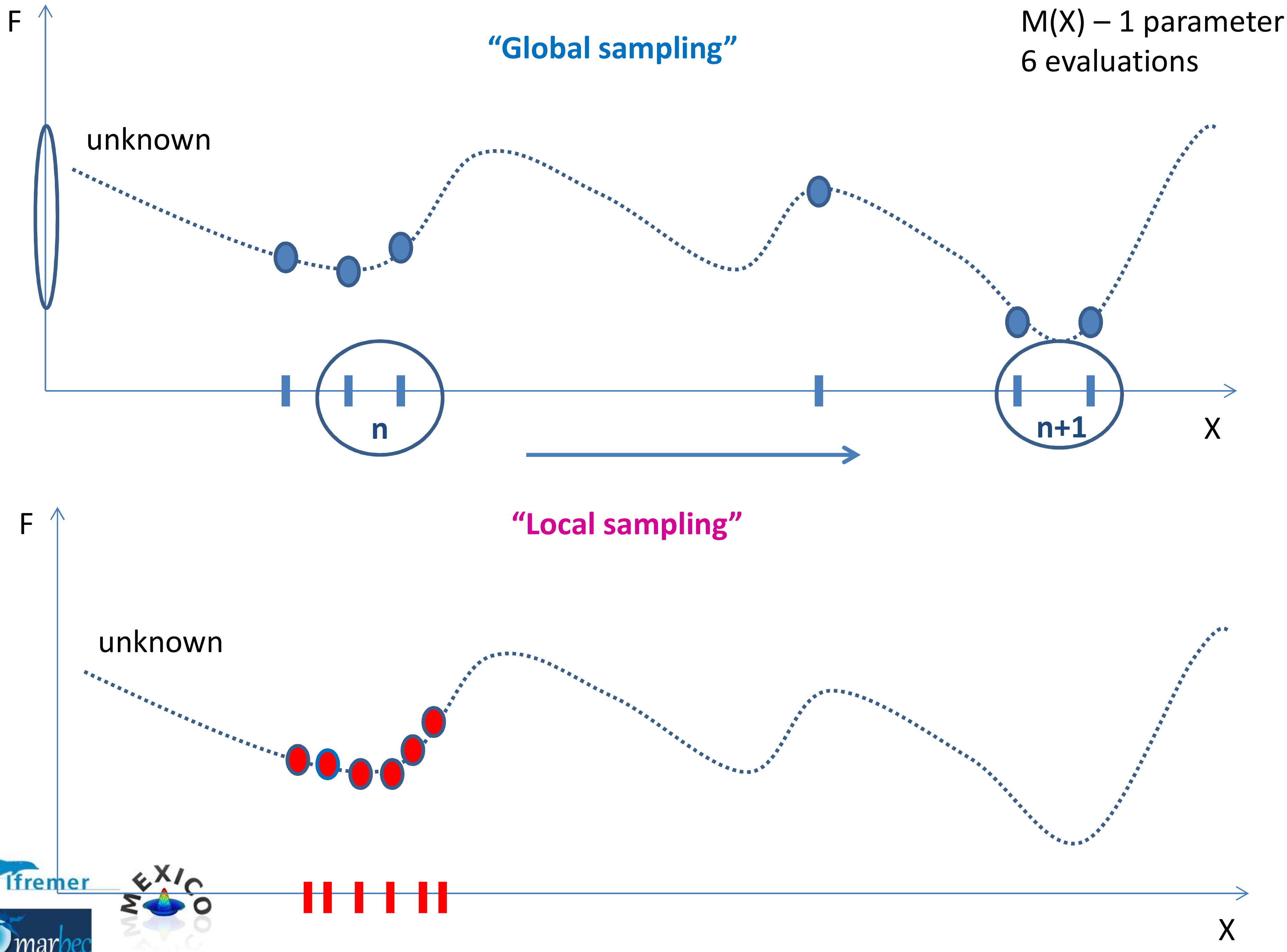
Numerical assessment of metamodelling strategies in computationally intensive optimization

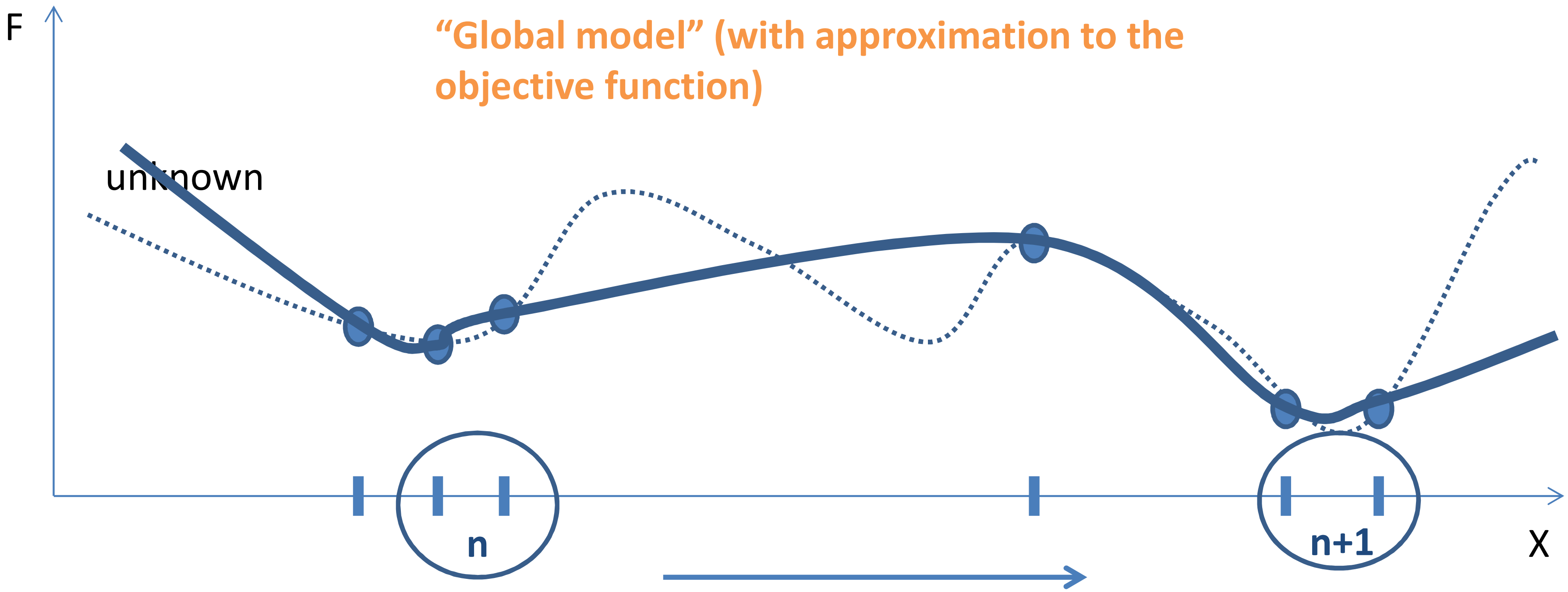
Saman Razavi*, Bryan A. Tolson, Donald H. Burn

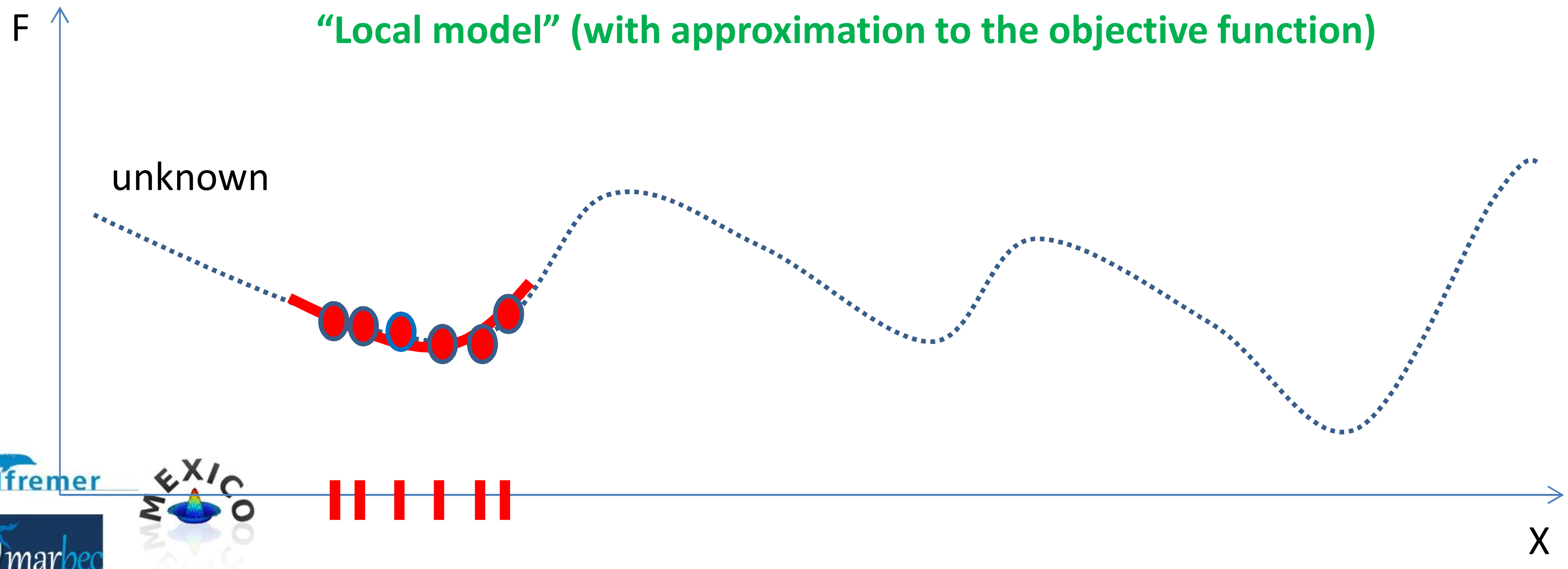
Which algorithm?

Abundant literature (highly technical, especially for computer scientists)

- Working with a mathematician (Rodolphe Leriche) and a computer scientist (Dimo Brockhoff)
- 4 large families (not so tight boundaries)
- 2 criteria :
  - Space exploration approach : local versus global
  - Sampling technic of parameters space : sampling versus model based (approximating the objective function)

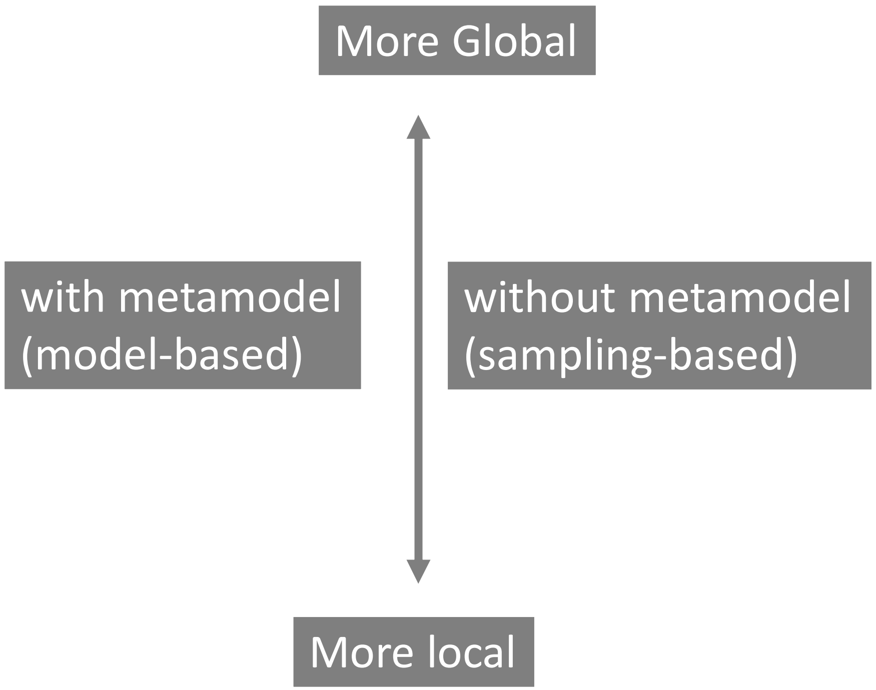

F
"Global sampling"
M(X) – 1 parameter
6 evaluations
unknown
n
n+1
X
F
"Local sampling"
unknown
X


"Global model" (with approximation to the objective function)
F
unknown
n
n+1
X

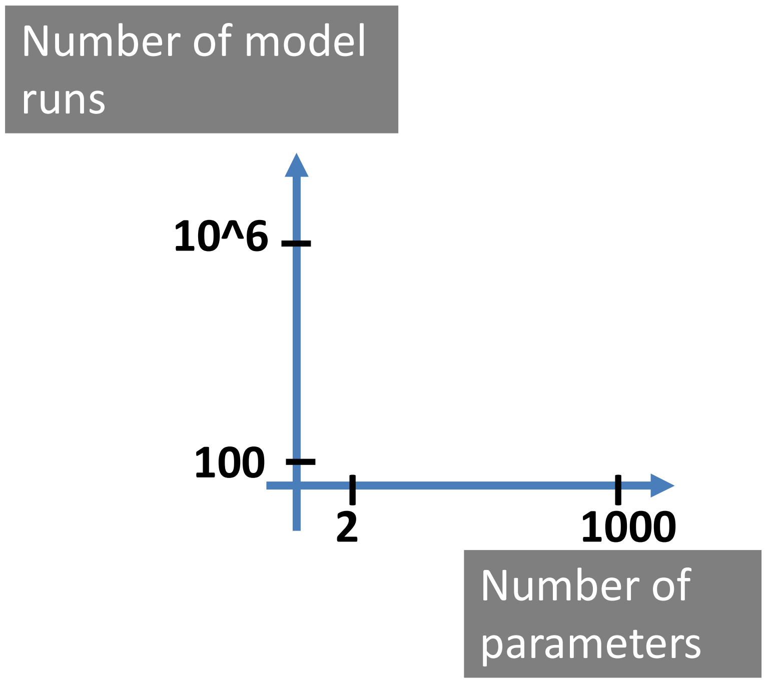

"Local model" (with approximation to the objective function)
F
unknown
X

Two grids to guide selection

Grid 1 : projection space



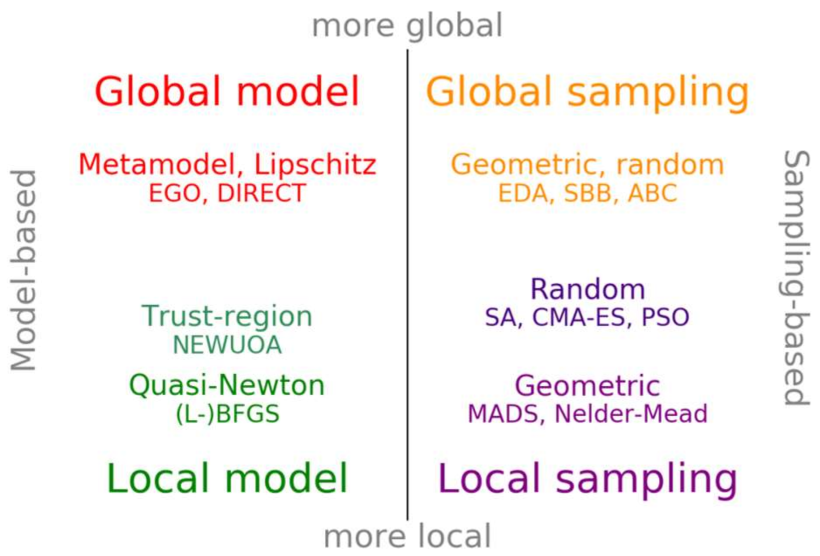
Grid 2: help in selecting



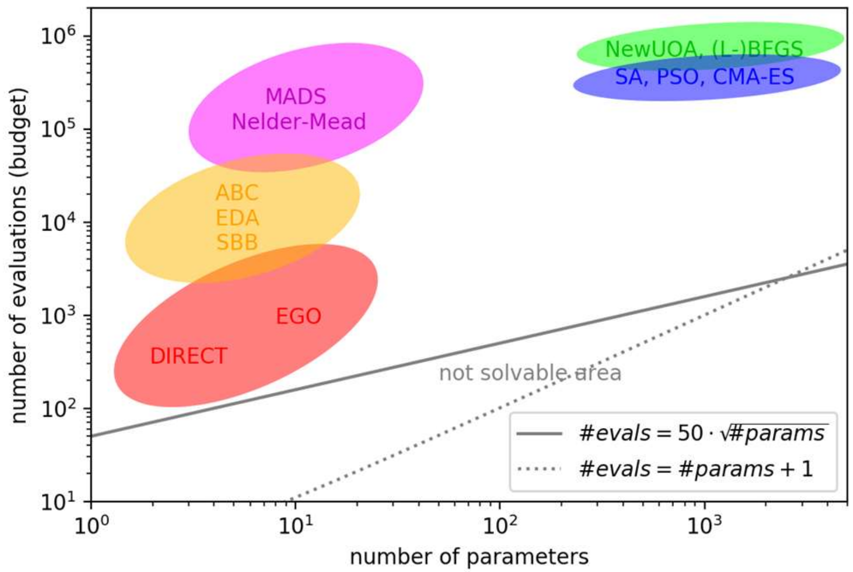
- **Grid 1 : position the different families in the space of the two criteria**
- **Grid 2 : help in selecting a family of optimization methods**

Two grids to guide selection

Grid 1 : projection space

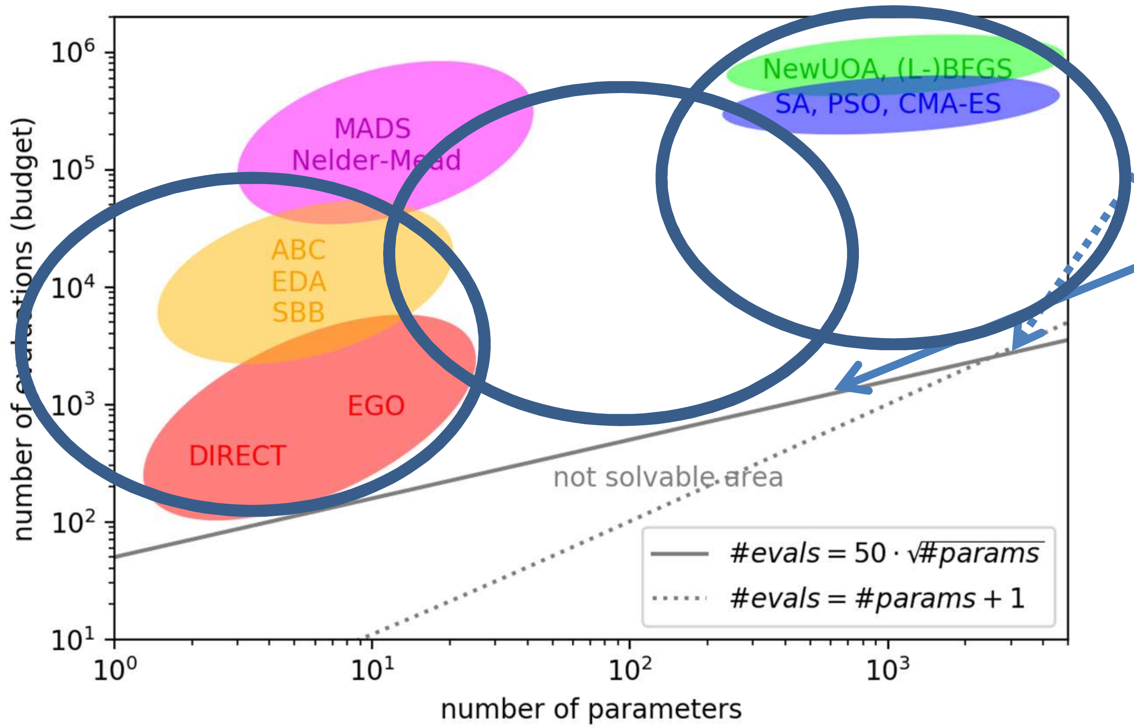


Grid 2: help in selecting



- **Grid 1 : position the different families in the space of the two criteria**
- **Grid 2 : help in selecting a family of optimization methods**

Grid : Parameters/Number of runs



Non-solvable linear problem

In general, unsolvable optimization problem

Who can do more can do less

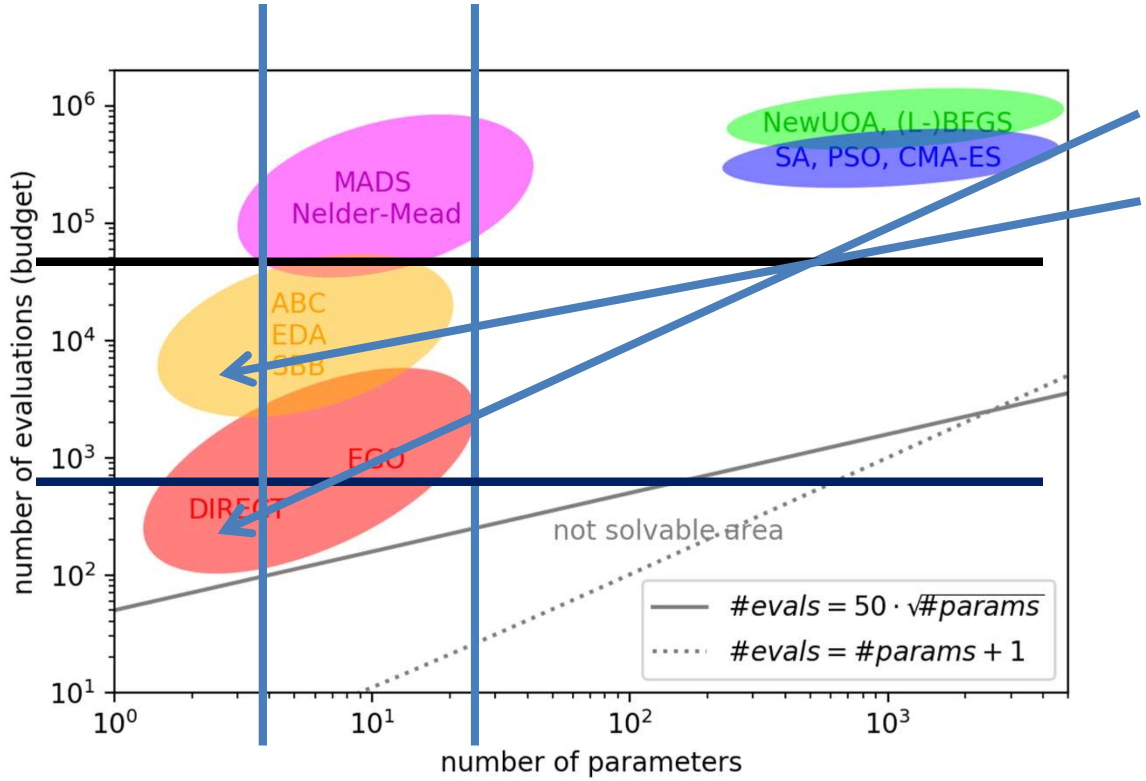
EGO : efficient global optimisation - Jones et al. (1998)
DIRECT : Dividing RECTangles – Jones et al 1993

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)

Grid : Parameters/Number of runs



Few parameters, few runs

Few parameters, more runs

A lot of parameters

EGO : efficient global optimisation - Jones et al. (1998)
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NEWUOA : (Powell 2006)
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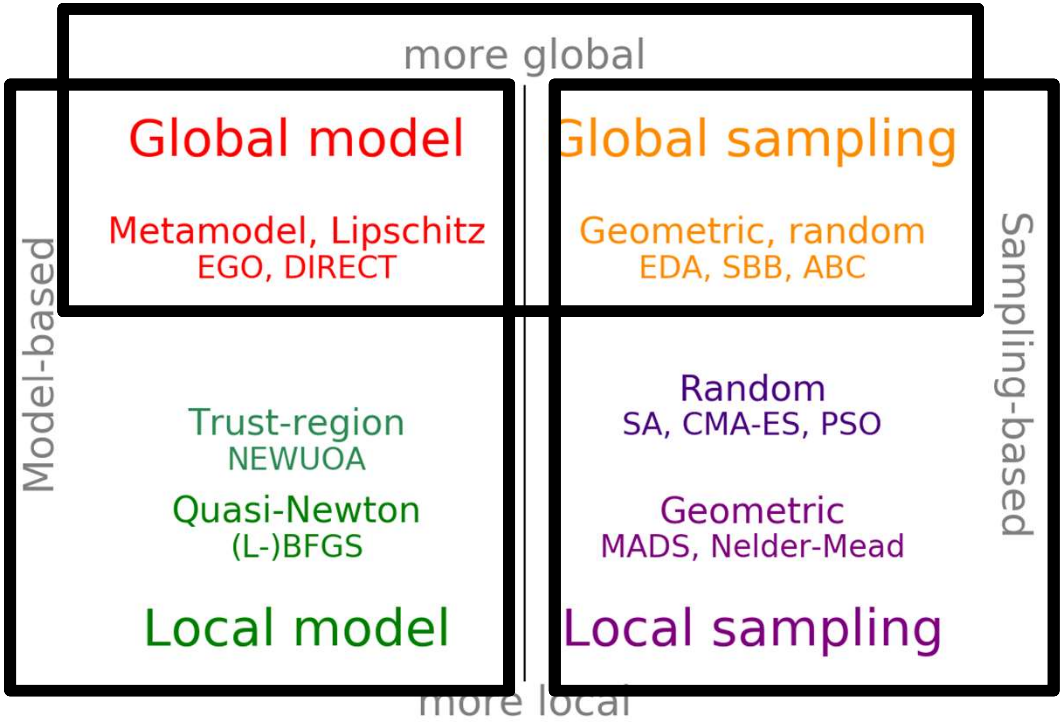
Nelder-Mead (Nelder et al 1965)

Grid 1 : Space explo./sampling



- **Algorithms with metamodel :** first- and second-order derivatives of the function around the optimum (optimum?, identifiability?, confidence intervals?)
- **Algorithms without metamodel :** family of solutions around the optimum (approximate form of the objective function and parameter covariances, distribution, etc.)
- Global exploration algorithms: approximate form of the objective function on the variable space (accuracy will depend on the balance between exploration and intensification phases)

Post-processing

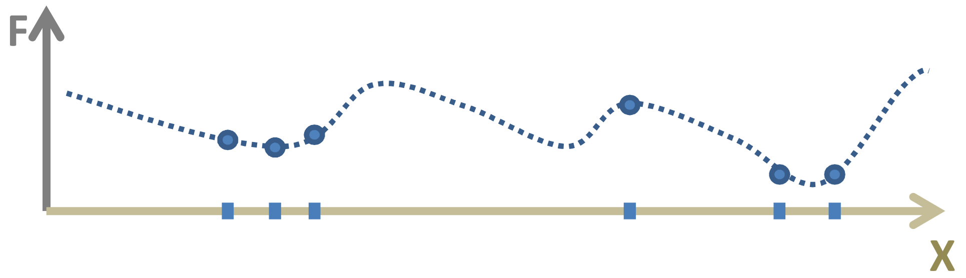
Some attempts, but few or no turnkey tools available

- Assessing optimization quality
  - convergence: “are we far from the minimum?”
  - global/local: “has the algorithm dipped into the local trough?”
  - parameter identifiability: “do several solutions give the same minimum?”
- Solving multi-criteria
- Stop or again?

For all algorithms

At each iteration, the algorithm calculates a set of solutions and the associated:

the trace of the algorithm in the space of X and in the space of F



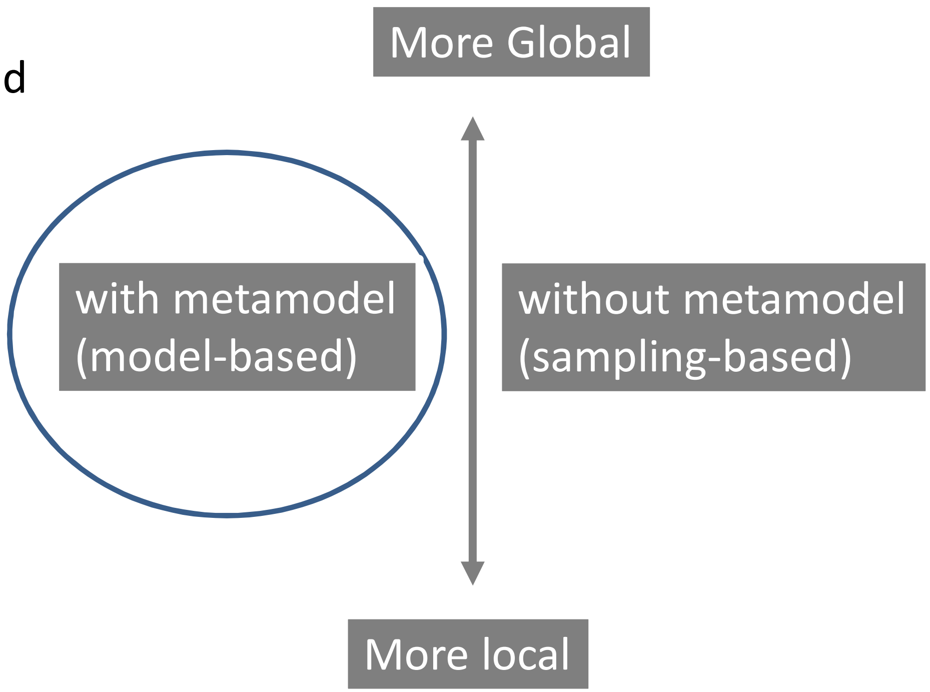
- **On X :** Oscillations, distances between solutions, dominant directions, frequencies,
- **On F:** Series of best solutions, (e.g. Maier et al 2014)
- Sensitivity to initial points
- Sensitivity analysis around the solution (e.g. Kleijnen and Sargent 2000)
- Understanding the properties of F: holes, barriers, plateaus, correlations (e.g. Wright 1932)

Objective function reformulation
Reparameterization
Change of algorithms or control parameters

Depending on the family of algorithms

- **Algorithms with metamodel:**

an approximation of the function, first- and second-order derivatives of the function around the optimum (optimum?, identifiability?, confidence intervals?) - Hessian (e.g. Gill et al., 1981)



Depending on the family of algorithms

- **Algorithms without metamodel :** give an optimum but also a family of solutions around the optimum (approximate the form of the objective function and parameter covariances, distribution ...) (e.g. Kendall and Nichols 2002)

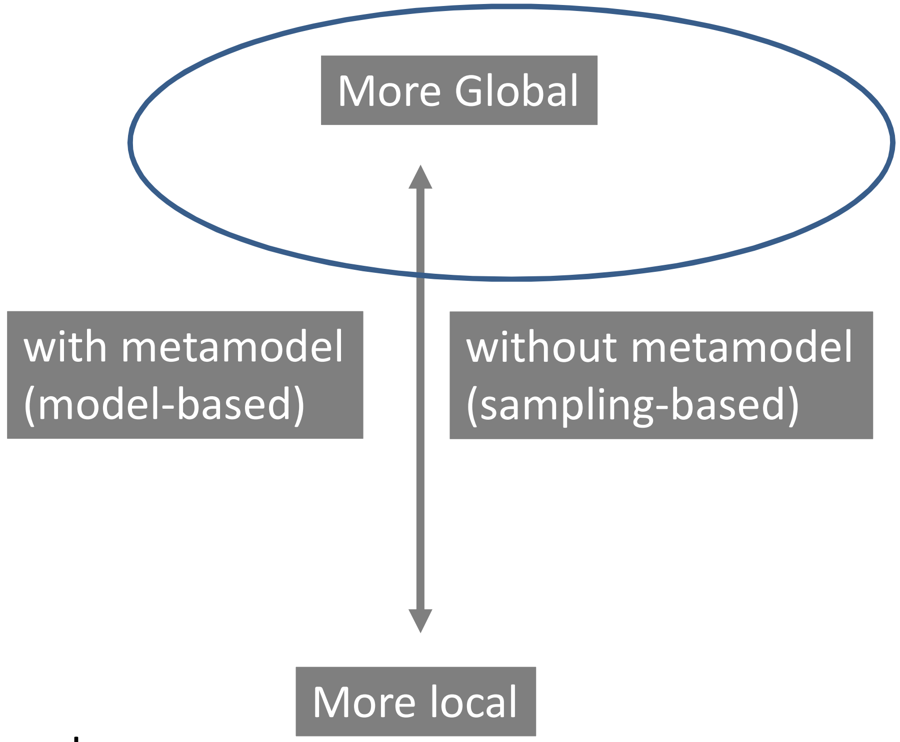
More Global

with metamodel (model-based)

without metamodel (sampling-based)

More local

Depending on the family of algorithms



- **Algorithms with global exploration:**
  capture an approximate form of the objective function on the variable space (accuracy will depend on the balance between the exploration and intensification phases)

Traceability, reproducibility and archiving

ODDO : Overview Description and Details of Optimization

In line with the famous ODD from 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	

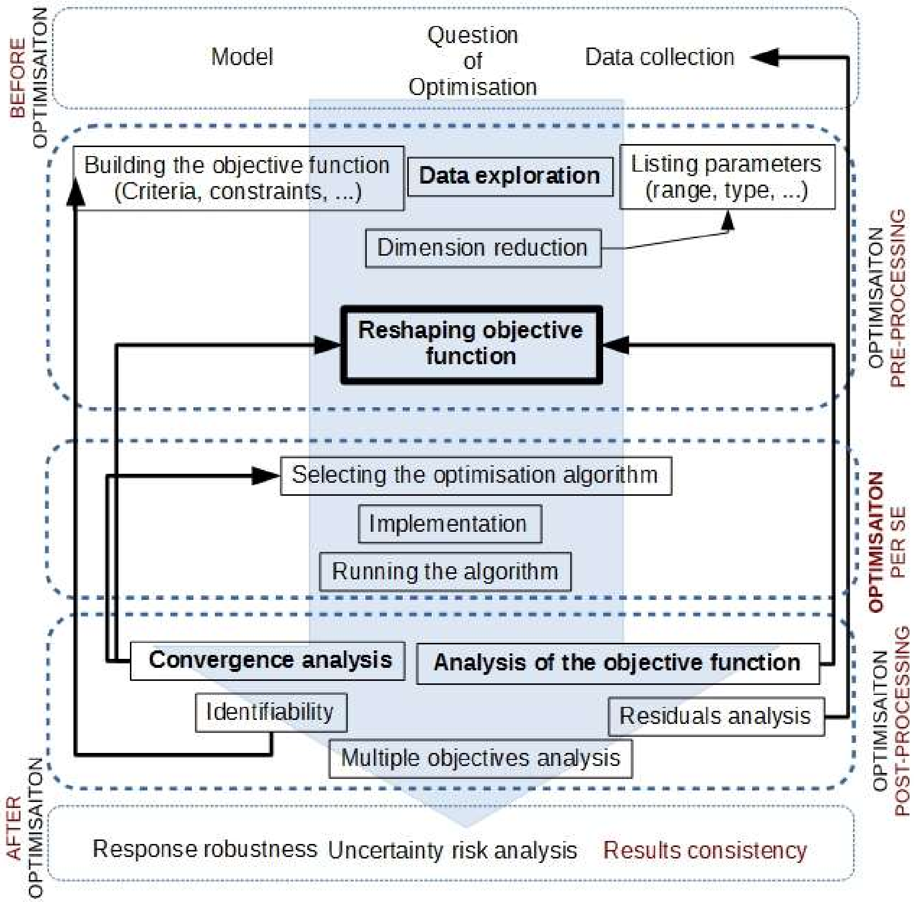
Algorithm	Family	
	Description-Justification	
	Changes in the algorithm	
	Settings	

Post-processing	Convergence	
	Optimum properties including Identifiability	
	Residual analysis	
	Multicriteria	

Comment	Number of simulations required	
	Duration	
	Reached stopping criteria	

In brief

Calibration : not such a linear approach



ODDO : Overview, Design, Details of Optimisation

(ODD Grimm 2010)

Pre-processing	Problem Formulation	Model	
		Question	
		Data	
		Parameters/ variables – Bounds&constrainsts	
		uncertainty	
		Initial objective function	
	Objective Fubction	building	
		reshaping	
		final	
	Exploratory Analysis	data	
		Reduction dimension	

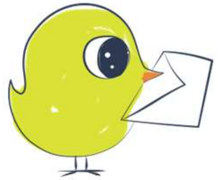
Algorithm	Family	
	Description-Justification	
	Adaptation	
	Settings	

Pos-processing	Convergence	
	Optimum properties	
	Identifiability	
	Residual analysis	
	Multicriteria	

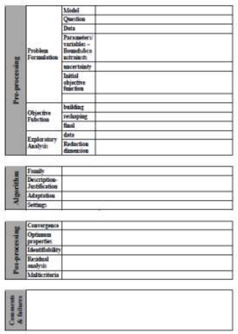
Comments & failures	

Recommendations

(slow science academy 2010)



mathematicians of numerical analysis / computer scientists



ODDO in Supplementary materials

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