Contact informations

Victor Trappler

PhD in applied mathematics (2021)

Title: *Parameter control in the presence of uncertainties*

with É. Arnaud, L. Debreu, A. Vidard

Keywords:

- Uncertainty Quantification
- Optimization under uncertainties
- Robust calibration of numerical models

Contact:

@ `victor.trappler@gmail.com`

`vtrappler.github.io`

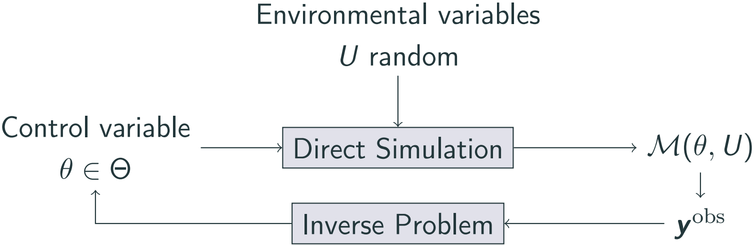
Research topics

1. Optimisation under Uncertainties
    - Notions of robustness in a calibration context
    - Regret-based family of estimators
2. Adaptive Strategies using GP to improve the estimations
    - GP formulation of the regret
    - SUR (Stepwise Uncertainty Reduction) strategies of design enrichment
    - AK-MCS (Adaptive Kriging Monte Carlo Sampling) for batch selection of points
3. Application: robust calibration of CROCO

Computer code and inverse problem

Input
- θ: Control parameter
- u: Environmental variables, realisations of r.v. U

Output
- $\mathcal{M}(\theta, u)$: Quantity to be compared to observations



Regret-based formulations

- $(\theta, u) \longmapsto J(\theta, u)$ objective function, *strictly positive*
- Best performance given u: $J^* : u \mapsto \min_{\theta \in \Theta} J(\theta, u)$

$\rightarrow$ Find $\hat{\theta}$ such that $J(\hat{\theta}, U)$ "close to" $J^*(U) = J(\theta^*(U), U)$ with high enough probability

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- Regret: $r(\theta, u) = J(\theta, u) - J^*(u)$ or $r(\theta, u) = \frac{J(\theta,u)}{J^*(u)}$
- $\Gamma_\alpha(\theta) = \mathbb{P}_U\left[r(\theta, U) \leq \alpha\right]$: Probability that the regret is below a level α, set by the user

Regret-based family of estimators (Trappler et al., 2020)

$$\left\{\hat{\theta} \mid \hat{\theta} = \operatorname*{arg\,max}_{\theta\in\Theta} \Gamma_\alpha(\theta), \alpha > 1\right\}$$

Adaptive strategies for the estimation of Γ_α

Let $Z \sim \mathrm{GP}(m_Z, C_Z)$ be a GP constructed on $\Theta \times \mathbb{U}$ based on J. We use Z to estimate Γ_α.

Several (myopic) strategies can be implemented:

- Reduction of the *augmented* IMSE of $\Delta = Z - \alpha Z^*$
- Improve estimation of the set $\{\Delta \leq 0\}$, using probability of coverage

Batch enrichment:

- Sampling in the margin of uncertainty of $\{\Delta \leq 0\}$, and transformations to get a batch of points (AK-MCS (Dubourg et al., 2011; Razaaly and Congedo, 2020))

Adaptive strategies for the quantile of the regret

Alternatively: what if α not fixed, but we are looking to reach a specific probability instead?

Under certain conditions, the ratio Z/Z^* is approximately log-normally distributed. Let us define $\Xi = \log Z/Z^*$

- Reduction of the augmented IMSE of Ξ
- Sampling in regions of interest, and subsequent transformations (QeAK-MCS (Razaaly, 2019))

Summary

Research topics (so far)

- Formulation of a notion of robustness using the regret
- Adaptive methods using GP for the estimation of Γ_α
- Application to the numerical model CROCO: robust estimation of the bottom friction

In progress

- Adaptive strategies for the *optimisation* (2-stage methods)
- Development of python package(s) for adaptive methods (based on scikit-learn)
- How to deal with realistic models ?
  - Expensive in terms of time and resources required
  - Dimension reduction

References i

Dubourg, V., Sudret, B., and Bourinet, J.-M. (2011). Reliability-based design optimization using kriging surrogates and subset simulation. *Structural and Multidisciplinary Optimization*, 44(5):673–690.

Razaaly, N. (2019). *Rare Event Estimation and Robust Optimization Methods with Application to ORC Turbine Cascade*. These de doctorat, Université Paris-Saclay (ComUE).

Razaaly, N. and Congedo, P. M. (2020). Extension of AK-MCS for the efficient computation of very small failure probabilities. *Reliability Engineering & System Safety*, 203:107084.

References ii

Trappler, V., Arnaud, É., Vidard, A., and Debreu, L. (2020). Robust calibration of numerical models based on relative regret. *Journal of Computational Physics*, page 109952.

“Most Probable Estimate”, and relaxation

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$$\theta^*(U) = \operatorname*{arg\,min}_{\theta \in \Theta} J(\theta, U)$$

$\longrightarrow$ estimate its density (how often is the value θ a minimizer)

$$p_{\theta^*}(\theta) = \text{"}\,\mathbb{P}_U \left[J(\theta, U) = J^*(U) \right]\text{"}$$

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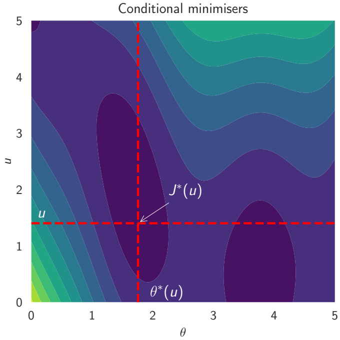
How to take into account values not optimal, but not too far either $\longrightarrow$ relaxation of the equality with $\alpha > 1$:

$$\Gamma_\alpha(\theta) = \mathbb{P}_U\left[J(\theta, U) \leq \alpha J^*(U)\right]$$

Relative-regret: illustration



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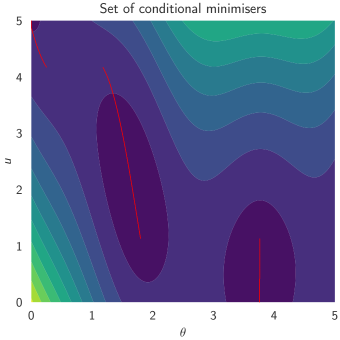
Relative-regret: illustration



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- Set of conditional minimisers: $\{(\theta^*(u), u) \mid u \in \mathbb{U}\}$

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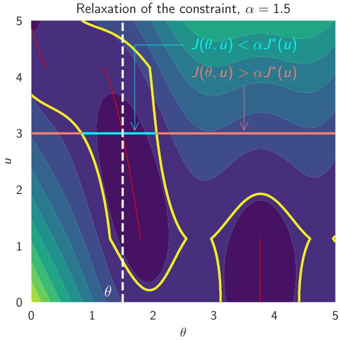

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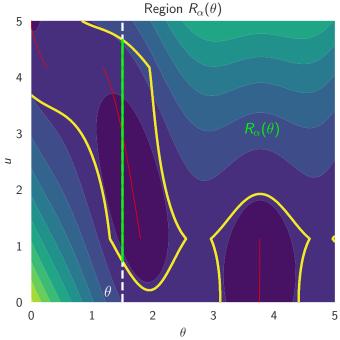


- Sample $u \sim U$, and solve $\theta^*(u) = \arg\min_{\theta \in \Theta} J(\theta, u)$
- Set of conditional minimisers: $\{(\theta^*(u), u) \mid u \in \mathbb{U}\}$
- Set $\alpha \geq 1$
- $R_\alpha(\theta) = \{u \mid J(\theta, u) \leq \alpha J^*(u)\}$
- $\Gamma_\alpha(\theta) = \mathbb{P}_U [U \in R_\alpha(\theta)]$

Getting an estimator

$\Gamma_\alpha(\theta)$: probability that the cost (thus θ) is α-acceptable

- If α known, maximize the probability that θ gives acceptable values:

$$\max_{\theta\in\Theta} \Gamma_\alpha(\theta) = \max_{\theta\in\Theta} \mathbb{P}_U \left[J(\theta, U) \leq \alpha J^*(U)\right] \tag{1}$$

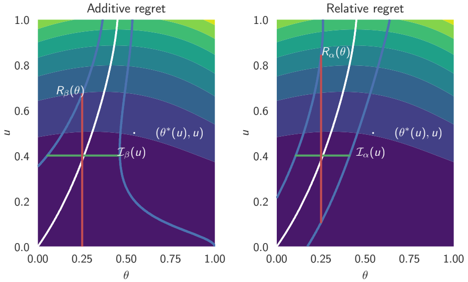
- Set a target probability $1-\eta$, and find the smallest α.

$$\inf\{\alpha \mid \max_{\theta\in\Theta} \Gamma_\alpha(\theta) \geq 1-\eta\} \tag{2}$$

Relative-regret family of estimators (Trappler et al., 2020)

$$\left\{\hat{\theta} \mid \hat{\theta} = \operatorname*{arg\,max}_{\theta\in\Theta} \Gamma_\alpha(\theta), \alpha > 1\right\} \tag{3}$$

Why the relative regret ?



- Relative regret
  - α-acceptability regions large for flat and bad situations ($J^*(u)$ large)
  - Conversely, puts high confidence when $J^*(u)$ is small
  - No units $\rightarrow$ ratio of costs

Notions of regret

Let $J^*(u) = \min_{\theta \in \Theta} J(\theta, u)$ and $\theta^*(u) = \arg\min_{\theta \in \Theta} J(\theta, u)$. The regret r:

$$r(\theta, u) = J(\theta, u) - J^*(u) = -\log\left(\frac{e^{-J(\theta,u)}}{\max_\theta\{e^{-J(\theta,u)}\}}\right) \tag{4}$$

$$= -\log\left(\frac{\mathcal{L}(\theta, u)}{\max_{\theta \in \Theta} \mathcal{L}(\theta, u)}\right) \tag{5}$$

$\rightarrow$ linked to misspecified LRT: maximize the probability of keeping $\mathcal{H}_0$: θ valid instead of $\arg\max \mathcal{L}$.

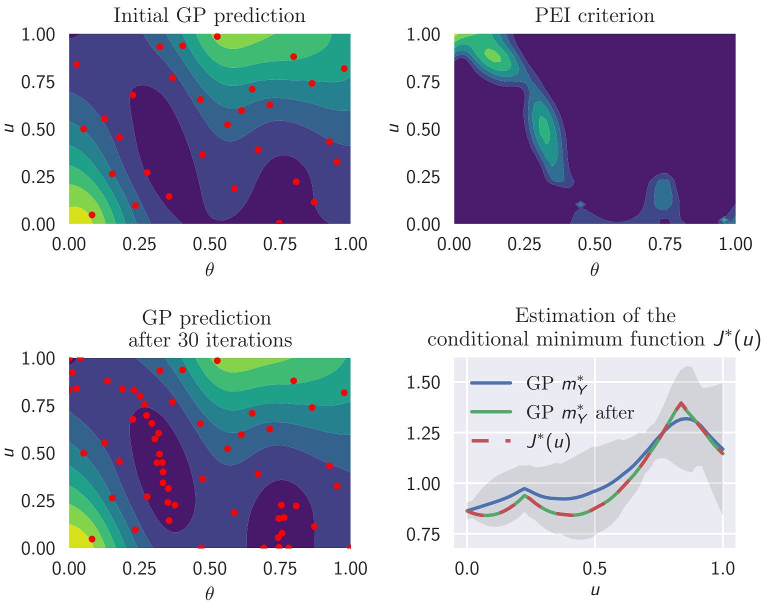
PEI criterion

$Z \sim \mathrm{GP}(m_Z, C_Z)$ on $\Theta \times \mathbb{U}$

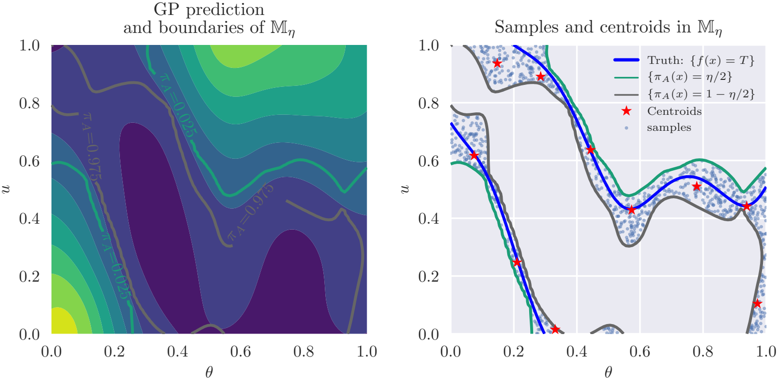
$$\mathrm{PEI}(\theta, u) = \mathbb{E}_{Z(\theta,u)}\left[\left[f_{\min}(u) - Z(\theta, u)\right]_+\right] \tag{6}$$

where $f_{\min}(u) = \max\left\{\min_i J(\theta_i, u_i), \min_{\theta\in\Theta} m_Z(\theta, u)\right\}$

Illustration of the PEI

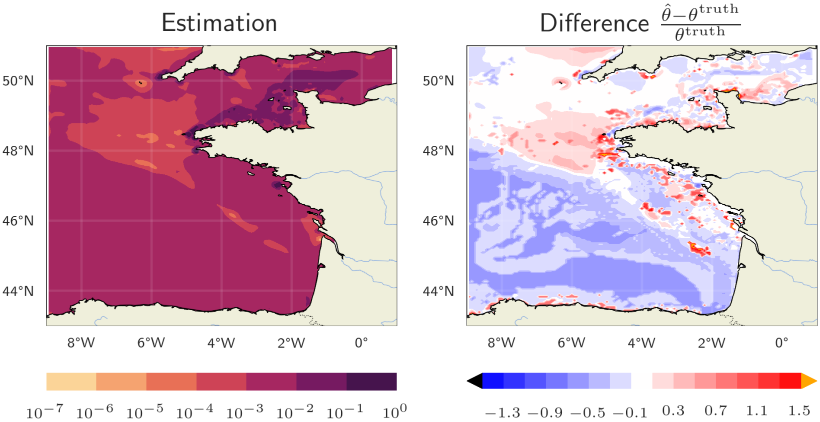


Principle of AK-MCS



An example: Misspecification of u

Minimization of $\theta \mapsto J(\theta, u)$, for different u, which parametrizes some boundary conditions: $u = (0.0, 0.0)$



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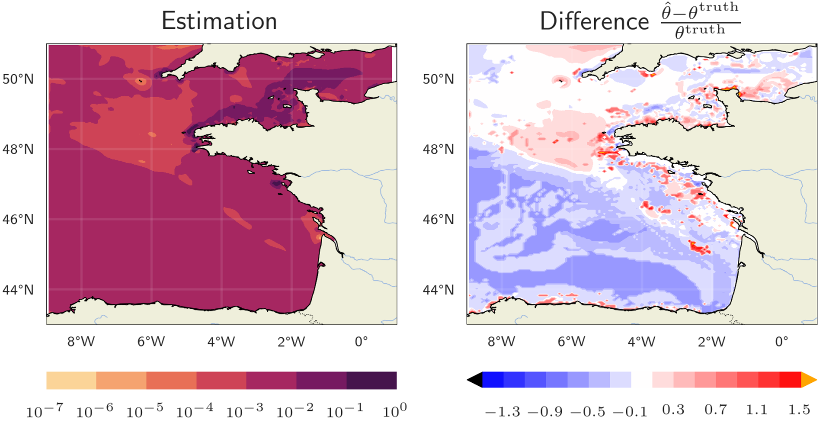
Minimization of $\theta \mapsto J(\theta, u)$, for different u, which parametrizes some boundary conditions: $u = (0.0, 0.5)$



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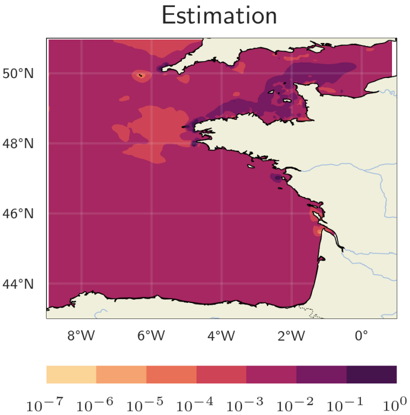

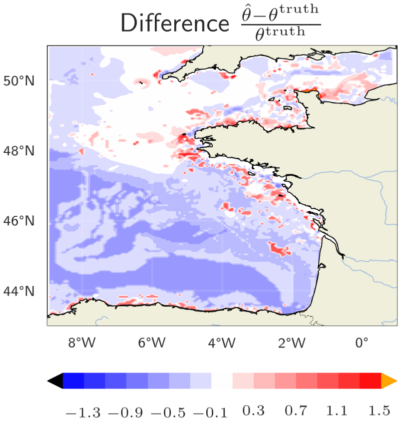

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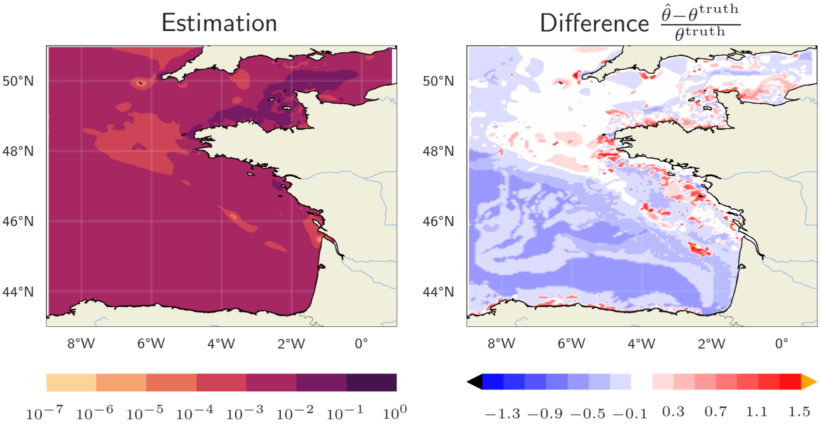
Minimization of $\theta \mapsto J(\theta, u)$, for different u, which parametrizes some boundary conditions: $u = (0.5, 0.0)$



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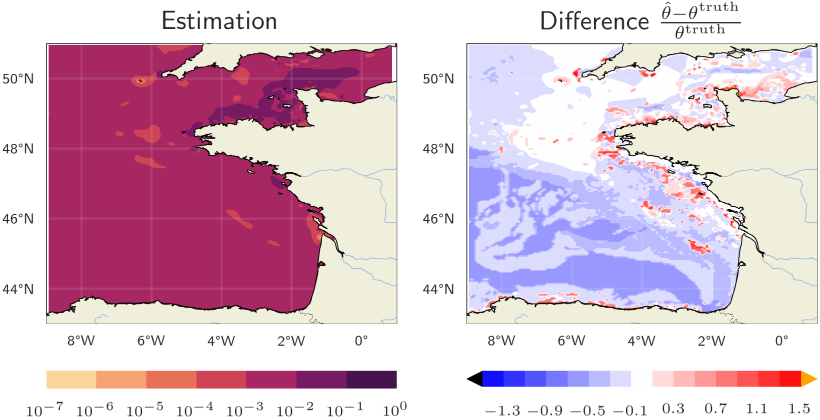

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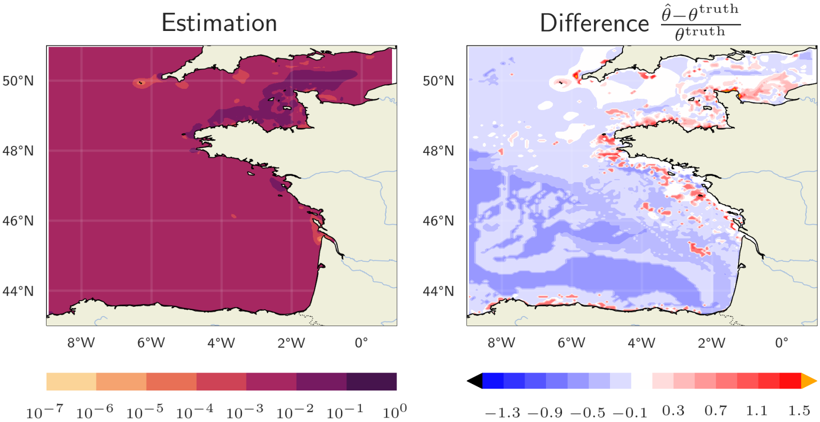

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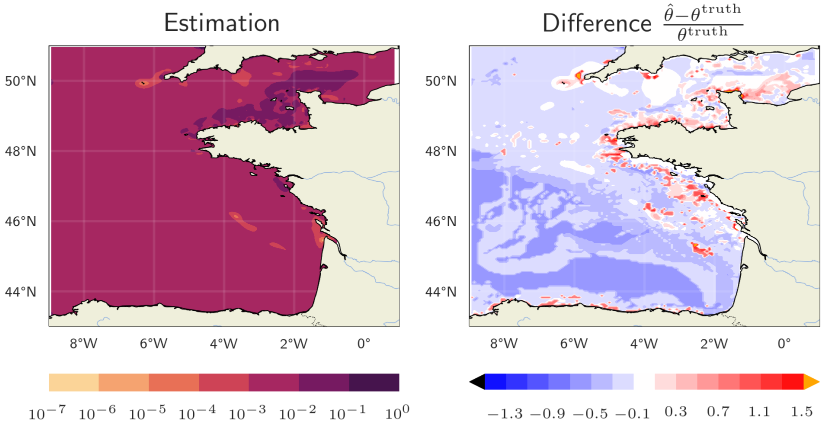

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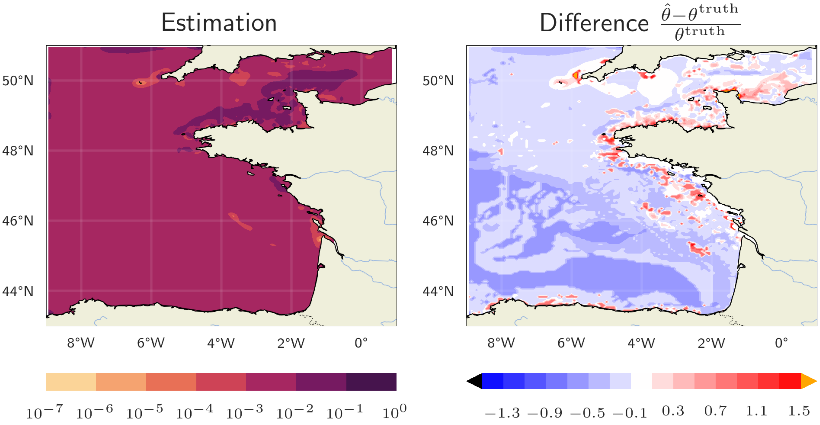

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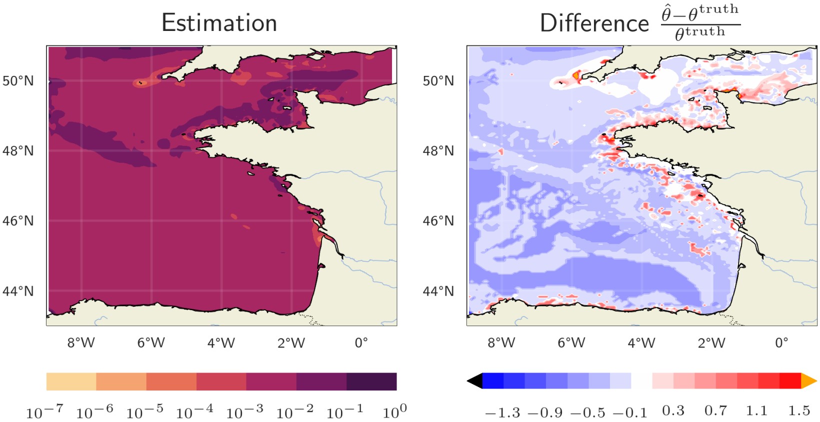

Conservative or optimistic estimate