Adaptive Surrogate Modeling for Bayesian Calibration with Model Disrepancy

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Workshop on Bayesian Optimization and related topics
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Presentation Outline

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Context

- Reliable simulations are needed in the context of nuclear engineering.
- The numerical code can be computationally expensive
- Multiple sources of uncertainty in numerical simulations: parameter uncertainty, model discrepancy, experimental uncertainty, code uncertainty.
- Need to account for these different sources of uncertainty in the calibration to improve the predictions

Goal: Performing robust calibration of model parameters considering model error for computationally expensive numerical codes

Presentation Outline

Bayesian calibration with model discrepancy

- Calibration consists on inferring the best values of the parameters to fit the observed data.

Statistical Assumptions

$$y_{obs}(x) = f(x, \theta) + \delta(x) + \varepsilon$$

- Model error is modeled as a Gaussian process $\delta(x)|GP(\mu(.), k_{\psi}(., .))$, the covariance function depends on some hyperparameters ψ
- Measurement error is distributed as $\mathcal{N}(0, \sigma_{\varepsilon}^2)$
- Prior distributions of the parameters and the hyperparameters

Bayesian calibration with model discrepancy

- Full Maximum a Posteriori (FMP) : Model discrepancy depends on model parameters [6].
- The hyperparameters $\phi = (\psi, \sigma_\varepsilon)$ are estimated by solving the following optimisation problem

$$\hat{\phi}_{FMP} = argmax(p(\phi|y,\theta)) = argmax\phi(x)(p(y|\phi,\theta)$$

- The posterior density of the parameters is estimated by

$$p(\theta,\phi|y_{obs}) \propto p(\theta)p(y_{obs}|\theta,\phi = \hat{\phi}_{FMP})$$

- We use Metropolis Hastings algorithm to sample from the posterior distribution.

Presentation Outline

Adaptive Surrogate Modeling: Gaussian Process Meta-Model

- A surrogate model is a statistical representation of the numerical code.
- It is cheaper to evaluate.

A priori

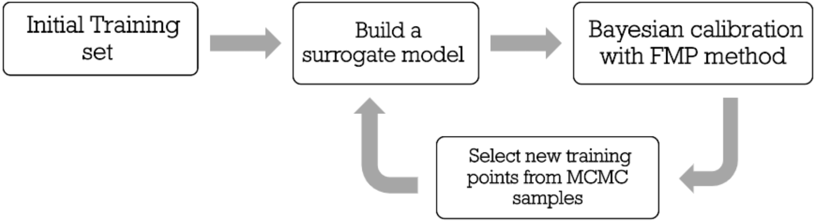
$$f_{code} \sim GP(m(.), K(.,.))$$

- $m(.)$ is the mean function
- $k(.,.)$ is the covariance function
- We consider a set of training inputs $X = (x_1, x_2, .., x_n)$ with their corresponding code outputs $Y = (y_1 = f_{code}(x_1), f_{code}(x_2), .., f_{code}(x_n))$
- Let $X_* = (x_{*,1}, x_{*,2}, .., x_{*,n})$ be the test set where we want to make the predictions and Y_* their corresponding outputs.
- We can predict Y_* by

$$Y_* | Y, X_*, X \sim \mathcal{N}(\mu_* - K_* K^{-1}(Y - \mu(X)), K_{**} - K_*^T K^{-1} K_*)$$

Adaptive Surrogate Modeling

- The idea is to minimize the Kullback-Leibler divergence from p_{FMP} to $\hat{p}_{FMP}$
- Place training points where posterior probability is high
- Reduce the number of observations used to build the surrogate.



Two approaches for selecting the new training points:

- Random samples from the MCMC chain
- Weighted sampling

Adaptive Surrogate Modeling

Algorithm 1 Adaptive construction of a surrogate model

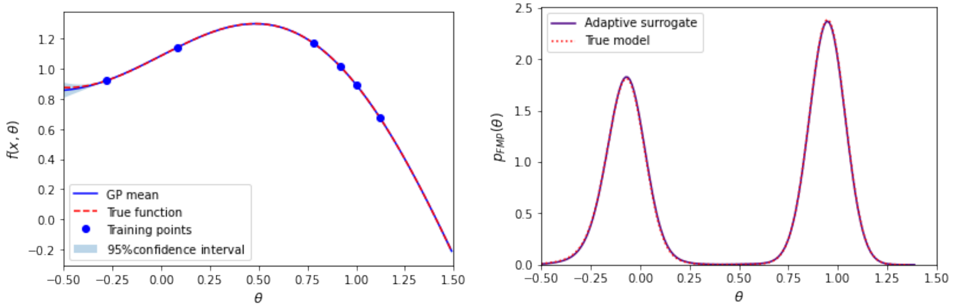
Create an initial DoE of size n_s
Construct a surrogate model $\hat{f}$ for the numerical code
Perform FMP calibration to find a posterior distribution $p(\theta)$
while $n < n_{max}$ **do**
    Select new design points from the posterior distribution
    Evaluate the model at the new set of points
    Update the surrogate $\hat{f}$
    Perform FMP calibration with the updated surrogate
end while

Adaptive Surrogate Modeling

Toy example 1 We consider the following function:

$$f(x,\theta) = xsin(2\theta x) + (x + 0.15)(1 - \theta)$$

with the true process modeled as $y(x) = x$



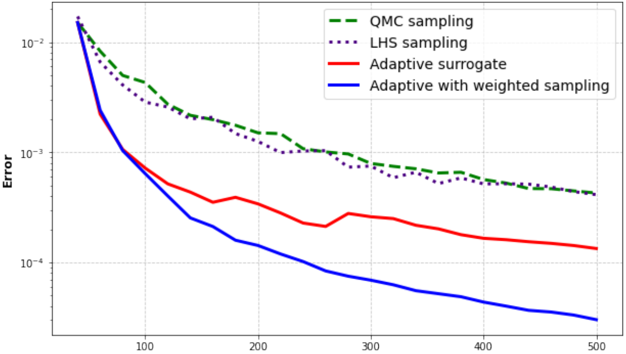
The left figure is the functions f with the training points, and the right figure is a comparison between the posterior distribution of the parameter θ with the true model and with the sequence of surrogates

Adaptive Surrogate Modeling

Toy example 2

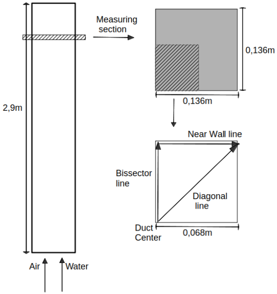
$$G(x, \theta) = \prod_{i=1}^{n} \frac{|4x_i - 2| + \theta_i}{1 + \theta_i}$$

We use 20 observations for the calibration from the true process with $\theta_{true} = (0.55, 0.8, 0.3, 0.04, 0.6, 0.9)$ and noise $\sigma^2 = 0, 05$



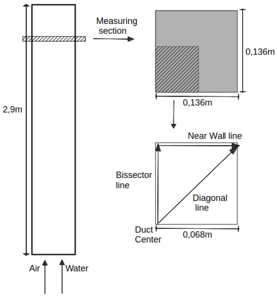
Presentation Outline

Application to the TRITON model

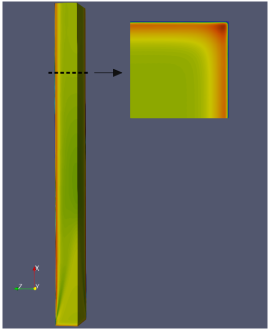


- Sun experiment : Development of gaz-liquid bubbly flow for a vertical square duct. [12]
- The case of $j_l = 0,5 m/s$, $j_g = 0.09 m/s$ and $\alpha_{gaz} = 0.139$

Application to the TRITON model



- Simulation with Neptune CFD using the TRITON (Two-phase RegIme TransitiON) model [2].



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Application to the TRITON model

- The TRITON model considers 3 fields: a continuous liquid field, a dispersed gaz field (group 1) and a continuous gaz field (group 2)
- Continuity and moment equations are solved for each field.
- The change in bubble diameters is described by the two-group interfacial area transport equations

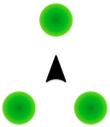
$$\frac{\partial a_{i1}}{\partial t} + \nabla.(a_{i1} v_{i1}) = \frac{2}{3}\frac{a_{i1}}{\alpha_{g1}}\left[\frac{\partial \alpha_{g1}}{\partial t} + \nabla.(\alpha_{g1} v_{g1})\right] - \chi\left(\frac{D_{sc}}{D_{sm}}\right)^2 \frac{a_{i1}}{\alpha_{g1}}\left[\frac{\partial \alpha_{g1}}{\partial t} + \nabla.(\alpha_{g1} v_{g1})\right] + \boxed{\sum_j \phi_{j,1}}$$

$$\frac{\partial a_{i2}}{\partial t} + \nabla.(a_{i2} v_{i2}) = \frac{2}{3}\frac{a_{i2}}{\alpha_{g2}}\left[\frac{\partial \alpha_{g2}}{\partial t} + \nabla.(\alpha_{g2} v_{g2})\right] + \chi\left(\frac{D_{sc}}{D_{sm}}\right)^2 \frac{a_{i1}}{\alpha_{g1}}\left[\frac{\partial \alpha_{g1}}{\partial t} + \nabla.(\alpha_{g1} v_{g1})\right] + \boxed{\sum_j \phi_{j,2}}$$

- For Bubbly flow,

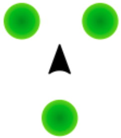
$$\sum_j \phi_j = \phi^1_{RC} + \phi^1_{WE} + \phi^1_{TI}$$

Application to the TRITON model



Random Collision: $C_{RC}^{(1)}$, C_{RC1}

Wake Entrainement : $C_{WE}^{(1)}$



Turbulent Impact: $C_{TI}^{(1)}$, We_{cr1}

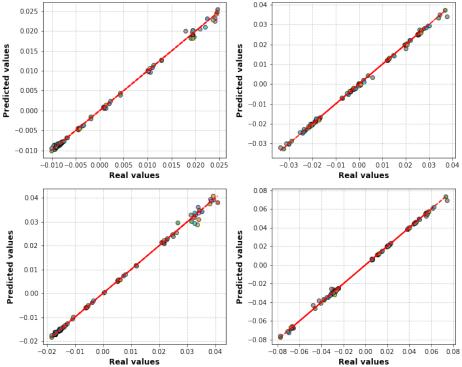
Based on One at A Time analysis, parameter ranges and priors are defined:

Parameter	Actual value	Prior	Range
$C_{RC}^{(1)}$	0.005	Log-Uniform	$[10^{-5}, 10^{-1}]$
C_{RC1}	3.0	Uniform	$[1, 4]$
$C_{WE}^{(1)}$	0.002	Log-Uniform	$[10^{-4}, 10^{-2}]$
We_{cr1}	6.5	Uniform	$[4., 7.]$
C_{TI}^{1}	0.1	Uniform	$[0.05, 0.15]$

Application to the TRITON model

Surrogate of Neptune CFD

- DoE of 50 training points generated using QMC Method and a test set of 10 points with LHS sampling.
- Gaussian Processes with mean 0 and seperated RBF kernel are used.
- Validation of the surrogate by calculating the normalized quadratic error for the validation set.

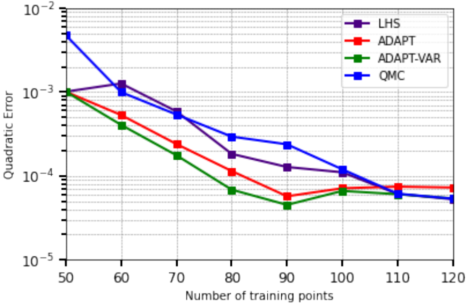


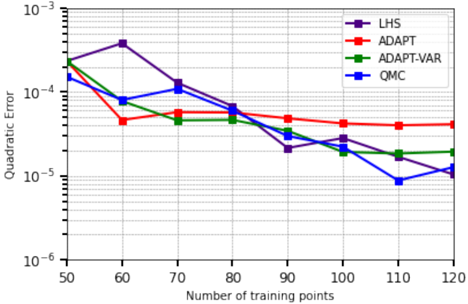
	α_d	α_b	α_n	W_d	W_b	W_n
Quadratic error	0,011	0,05	0,036	0,01	0,038	0,034

Application to the TRITON model

Adaptive Surrogate of Neptune CFD

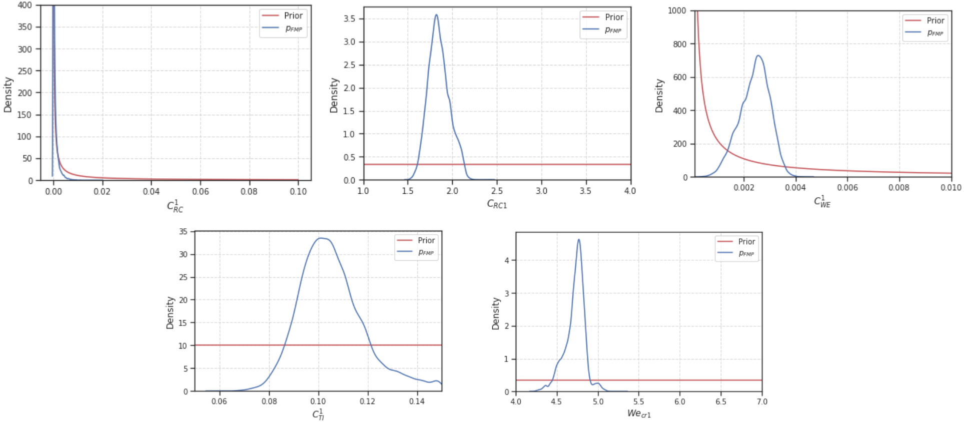
- The adaptive approach is applied to the surrogate of the numerical code.
- Convergence of the approach:





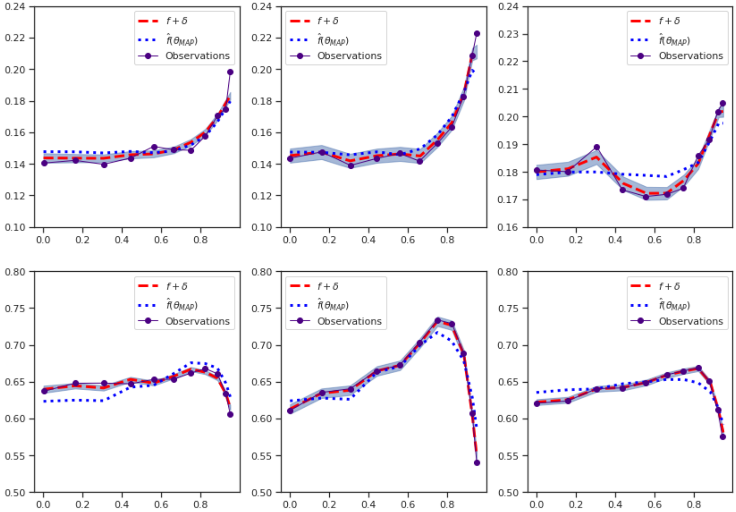
Application to the TRITON model

The Posterior density of the parameters



Application to the TRITON model

Predictions of the void fraction (Top row) and the liquid velocity (bottom row)



Presentation Outline

Conclusion

- An adaptive approach for surrogate construction of the numerical code.
- Application of the strategy to calibrate a complex two-phase flow model.
- Characterisation of model error and experimental uncertainty.

Perspectives

- Application to more complex cases
- Considering new forms of model error
- Design of physical experiments

Thank you for your attention!
Any questions?

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References I

[1] Maria J Bayarri et al. “A Framework for Validation of Computer Models”. en. In: *Technometrics* 49.2 (May 2007), pp. 138–154. DOI: 10.1198/004017007000000092.

[2] Clément Bazin. “Numerical and experimental studies of two-phase flows interacting with a bundle of tubes”. In: ().

[3] Dave Higdon et al. “Combining Field Data and Computer Simulations for Calibration and Prediction”. en. In: *SIAM Journal on Scientific Computing* 26.2 (Jan. 2004), pp. 448–466. DOI: 10.1137/S1064827503426693.

[4] Marc C. Kennedy and Anthony O’Hagan. “Bayesian calibration of computer models”. en. In: *Journal of the Royal Statistical Society: Series B (Statistical Methodology)* 63.3 (2001), pp. 425–464. DOI: 10.1111/1467-9868.00294.

References II

[5] E.V. Kuidjo Kuidjo et al. “Comparison of bubbles interaction mechanisms of two-group Interfacial Area Transport Equation model”. en. In: *International Journal of Multiphase Flow* 163 (June 2023), p. 104399. DOI: 10.1016/j.ijmultiphaseflow.2023.104399.

[6] Nicolas Leoni et al. “BAYESIAN CALIBRATION WITH ADAPTIVE MODEL DISCREPANCY”. en. In: *International Journal for Uncertainty Quantification* 14.1 (2024), pp. 19–41. DOI: 10.1615/Int.J.UncertaintyQuantification.2023046331.

[7] Jinglai Li and Youssef M. Marzouk. “Adaptive construction of surrogates for the Bayesian solution of inverse problems”. In: *SIAM Journal on Scientific Computing* 36.3 (Jan. 2014), A1163–A1186. DOI: 10.1137/130938189.

[8] Didier Lucor and Olivier P. Le Maître. “Cardiovascular Modeling With Adapted Parametric Inference”. en. In: *ESAIM: Proceedings and Surveys* 62 (2018). Ed. by Muhammad Dauhoo et al., pp. 91–107. DOI: 10.1051/proc/201862091.

References III

[9] Matthew Plumlee. “Bayesian Calibration of Inexact Computer Models”. en. In: *Journal of the American Statistical Association* 112.519 (July 2017), pp. 1274–1285. DOI: 10.1080/01621459.2016.1211016.

[10] Carl Edward Rasmussen and Christopher K. I. Williams. *Gaussian processes for machine learning*. en. Adaptive computation and machine learning. Cambridge, Mass: MIT Press, 2006.

[11] Thomas J. Santner, Brian J. Williams, and William I. Notz. *The Design and Analysis of Computer Experiments*. en. Springer Series in Statistics. New York, NY: Springer New York, 2003. DOI: 10.1007/978-1-4757-3799-8.

[12] Haomin Sun et al. “Upward air–water bubbly flow characteristics in a vertical square duct”. en. In: *Journal of Nuclear Science and Technology* 51.3 (Mar. 2014), pp. 267–281. DOI: 10.1080/00223131.2014.863718.