



# Inverse uncertainty quantification applied to thermal-hydraulic simulations

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DE LA RECHERCHE À L'INDUSTRIE



# Inverse uncertainty quantification applied to thermal-hydraulic simulations

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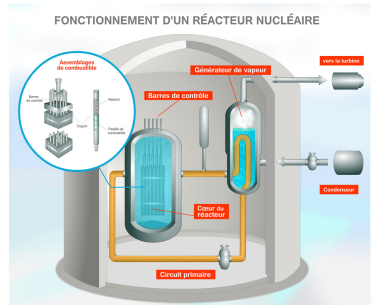
Statistics seminar in Rochebrune

26/03/2018

- 1 Motivations for inverse UQ in TH simulations
- 2 The CIRCE method
- 3 The Bayesian counterpart of CIRCE
- 4 Non linear generalization
- 5 Conclusions

Motivations for inverse UQ in TH simulations

- Best Estimate thermal-hydraulic system code developed by CEA,
- Based on six balance equations: mass, momentum and energy conservation
  - require building **correlations** (also called closure laws or physical models)
- Nuclear simulations with several levels of complexity:
  - Separate/Combined Effects Test (SET, CET)
    - at reduced scale, few physical phenomena
  - Integral Effect Test (IET)
    - many phenomena together.
- Simulating accidental transients for safety analysis
- Great effort devoted to V&V implementation
  - Verification : Are the equations solved right ?
  - Validation : Are the right equations solved ?



## CONCEPTION OF CORRELATIONS

- ex: heat transfers (convection, condensation, etc):

$$C_{nom}(\mathbf{x}, \theta)$$

where  $\mathbf{x}$  is a vector of physical variables and  $\theta$  is a fitting parameter.

- parameter uncertainty affecting  $\theta$  (neglected by physicists)

## V&V IMPLEMENTATION

- Verification stage : numerical uncertainties (ex: mesh convergence)
- Validation stage : where CATHARE 2 predictions are confronted to experimental data from SET.
  - correlation uncertainty assessed from differences between both of them  
 $\Rightarrow$  **inverse UQ process**

The CIRCE method

## MAIN ASSUMPTIONS

- Model uncertainty is multiplicative:

$$C_{\Lambda}(\mathbf{x}) = \Lambda \times C_{nom}(\mathbf{x})$$

- $\Lambda$  follows a probability distribution
- $\Lambda$  is log-Gaussian, calculated by the **CIRCE method** (De Crécy and Bazin, 2001).



CIRCE = *Calcul des Incertitudes Relatives aux Corrélations Élémentaires*.

## STATISTICAL MODELING

- $z_i \in \mathbb{R}$  the QoI experimentally measured at  $\mathbf{x}_i \in \mathbb{R}^m$
- $Y(\cdot)$  the CATHARE 2 code (used as a black-box function)
- For  $i \in \llbracket 1; n \rrbracket$ , we assume that

$$\begin{aligned} z_i &= Y(C_{\lambda_{1,i}}(\mathbf{x}_i), \dots, C_{\lambda_{p,i}}(\mathbf{x}_i)) + \epsilon_i \\ &= Y_{(\lambda_{1,i}, \dots, \lambda_{p,i})}(\mathbf{x}_i) + \epsilon_i \end{aligned}$$

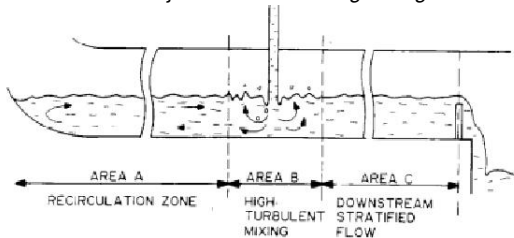
where

- $\lambda_{j,i} \sim \Lambda_j = \mathcal{LN}(m_j, \sigma_j^2)$ ,  $j \in \llbracket 1; p \rrbracket$
- $\alpha_{j,i} = \log(\lambda_{j,i}) \sim A_j = \mathcal{N}(m_j, \sigma_j^2)$ ,
- $\epsilon_i \sim \mathcal{N}(0, \sigma_{\epsilon_i}^2)$ .

The CIRCE method consists in estimating  $m_j$  and  $\sigma_j^2$  for  $j \in \llbracket 1; p \rrbracket$

## Ex: condensation flow rate at the safety injection

*Cooled water injected in the cold leg during LOCA*



- One correlation per area,
- We focus on area *B* and *C*,
- Condensation higher in the area *B* than area *C*,
- $Q_i$  = condensation flow rate measurement to the edge of area *C* ( $kg/s$ ),

■ The CATHARE 2 code can predict  $Q$  by using two correlations of condensation  $C_{\lambda_1}(\mathbf{x}_i)$  (area *B*) and  $C_{\lambda_2}(\mathbf{x}_i)$  (area *C*)

■  $Q_i = Y_{(\lambda_1, i, \lambda_2, i)}(\mathbf{x}_i) + \epsilon_i$   
where  $\mathbf{x}_i$  includes injection pressure, injection temperature, water height in the cold leg, etc.

## OTHER ASSUMPTIONS UNDERLYING CIRCE:

- The factors are not correlated each other:  $Cov(\Lambda_j, \Lambda_k) = 0$  ;  $1 \leq j \neq k \leq p$ ,
- The experimental variances  $\sigma_{\epsilon_i}^2$  are assumed known.

---

## CIRCE IMPLEMENTATION:

1. Linearization at  $\alpha_{nom} = \log(\lambda_{nom})$ , typically at the nominal model  $\mathbf{0}_p = \log \mathbf{1}_p$ 
  - $z_i - Y_i^{nom} = h_i^T(\alpha_i - \alpha_{nom}) + \epsilon_i$  with  $\alpha_i := \log \lambda_i$
  - Identifiability:  $\text{rank}(H) = p$  where  $H = [h_1, \dots, h_n]^T \in \mathcal{M}_{np}$ .
2. Computation of MLE estimates  $(\hat{m}_j, \hat{\sigma}_j^2)$  using an EM algorithm:
  - Both E and M steps are explicit,
  - ECME to speed up the convergence (Celeux et al., 2010).
3. Post treatment:
  - Statistical analysis of residuals, LOO cross validation,
  - Check the linearity assumption on

$$\text{IF}_{0.95}(A_j) = [\hat{m}_j - 1.96\hat{\sigma}_j, \hat{m}_j + 1.96\hat{\sigma}_j], \quad j \in \llbracket 1; p \rrbracket,$$

- Deduce the 95%-interval of  $\Lambda_j$  :  
 $\text{IF}_{0.95}(\Lambda_j) = [\exp(\hat{m}_j - 1.96\hat{\sigma}_j), \exp(\hat{m}_j + 1.96\hat{\sigma}_j)], \quad j \in \llbracket 1; p \rrbracket$

The Bayesian counterpart of CIRCE

## Notations:

- $\mathbf{z} = [z_1, \dots, z_n]^T \in \mathbb{R}^n$  the matrix of field measurements
- $\alpha = [\alpha_1, \dots, \alpha_n]^T \in \mathcal{M}_{np}$  the matrix of missing model log-samples:
- $m = (m_1, \dots, m_p)^T \in \mathbb{R}^p$  and  $\sigma^2 = (\sigma_1^2, \dots, \sigma_p^2)^T \in \mathbb{R}^p$ .

## STATISTICAL MODEL

- $z_i = h_i^T \alpha_i + \epsilon_i$  for  $i \in \llbracket 1; n \rrbracket$ ,
  - $z_i \in \mathbb{R}^q$ ;  $h_i \in \mathbb{R}^p$ ;  $\alpha_i \sim \mathcal{N}(m, \sigma^2) \in \mathbb{R}^p$ ;

## POSTERIOR DISTRIBUTION

- Bayes formula gives  $[m, \sigma^2 | \mathbf{z}, \alpha] \propto [\mathbf{z}, \alpha | \sigma^2, m][m, \sigma^2]$ 
  - Likelihood:  $\mathbf{z} | \alpha, \sigma^2, m \sim \otimes_{i=1}^n \mathcal{N}(h_i^T \alpha_i, R_i)$ ,
  - Prior:  $[m, \sigma^2] = [m | \sigma^2][\sigma^2]$ 
    - Conjugate Gaussian-inverse-gamma,
    - Gaussian for  $m | \sigma^2$  along with a folded non-standardized-t for  $\sigma$  (Gelman, 2006).

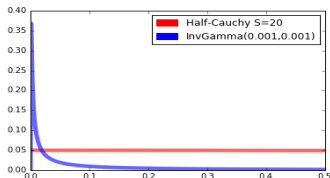
## INVERSE-GAMMA ( $\epsilon, \epsilon$ ) FOR $\sigma_j^2$

- Leads to an improper posterior as  $\epsilon \rightarrow 0$ .
  - Spiegelhalter et al. (2004) took  $\epsilon = 0.001$ ,
  - Inference is sensible to  $\epsilon$  (mainly when low values of  $\sigma$  provide large likelihood values),
  - Such diffuse priors cannot fix troubles with improper posteriors (Kass and Wasserman, 1996).

## FOLDED NON-STANDARDIZED STUDENT DISTRIBUTION FOR $\sigma_j$ (via the augmented model)

- $z_i = h_i^T \times (C\tilde{\alpha}_i) + \epsilon_i$  for  $i \in \llbracket 1; n \rrbracket$ , with  $\alpha_i = C\tilde{\alpha}_i$ 
  - Priors:  $C \sim \mathcal{N}(m_C, 1)$  and  $\sigma_{\tilde{\alpha}}^2 \sim \mathcal{IG}(0.5 \times \nu, S)$
  - Thus,  $\sigma = |C|\tilde{\sigma}$  is a folded noncentral-t
    - half-t if  $m_C = 0$ ,
    - half Cauchy if  $m_C = 0$  and  $\nu = 1$  (which tends to be uniform on  $\mathbb{R}^+$  as  $S \rightarrow +\infty$ )

$$[\sigma] \propto \frac{1}{\sigma^2 + S}$$



## SUBSTITUTION (OR DATA-AUG.) SAMPLING (Gelfand and Smith, 1990)

By following the hierarchical structure  $[m, \sigma^2, \alpha | \mathbf{z}] = [m, \sigma^2 | \alpha, \mathbf{z}][\alpha | \mathbf{z}]$

- Start with a first sample  $(m_0, \sigma_0^2)$
- In a loop  $k \geq 1$ , sample until convergence :
  1.  $\alpha_k \sim \alpha | \mathbf{z}, m_{k-1}, \sigma_{k-1}^2$  (Gaussian),
  2.  $m_k, \sigma_k^2 \sim m, \sigma^2 | \alpha_k, \mathbf{z}$  (Gaussian-inverse-gamma).

## GIBBS SAMPLING

Based on the full conditional posterior distributions

- Start with a first sample  $(m_0, \sigma_0^2)$
- In a loop for  $k \geq 1$ , sample until convergence :
  1.  $\alpha_k \sim \alpha | \mathbf{z}, m_{k-1}, \sigma_{k-1}^2$  (Gaussian),
  1.  $m_k \sim m | \sigma_k^2, \alpha_k, \mathbf{z}$  (Gaussian),
  2.  $\sigma_k^2 \sim \sigma^2 | b_k, \alpha_k, \mathbf{z}$  (inverse-gamma),

## SUBSTITUTION (OR DATA-AUG.) SAMPLING (Gelfand and Smith, 1990)

Full posterior  $[\tilde{m}, \tilde{\sigma}^2, \tilde{\alpha}, C | \mathbf{z}] = [\tilde{m}, \tilde{\sigma}^2 | \tilde{\alpha}, \mathbf{z}, C][\tilde{\alpha}, C | \mathbf{z}]$

- Start with a first sample  $(\tilde{m}_0, \tilde{\sigma}_0^2, C_0)$
- In a loop for  $k \geq 1$ , sample until convergence :
  1.  $\tilde{\alpha}_k \sim \tilde{\alpha} | \mathbf{z}, \tilde{m}_{k-1}, \tilde{\sigma}_{k-1}^2, C_{k-1}$  (Gaussian),
  2.  $C_k \sim C | \mathbf{z}, \tilde{\alpha}_k$  (Gaussian),
  3.  $\tilde{m}_k, \tilde{\sigma}_k^2 \sim \tilde{m}, \tilde{\sigma}^2 | \tilde{\alpha}_k, \mathbf{z}, C_k$  (Gaussian-inverse-gamma).

## GIBBS SAMPLING

Based on the full conditional posterior distributions:

- Start with a first sample  $(\tilde{m}_0, \tilde{\sigma}_0^2, C_0)$
- In a loop for  $k \geq 1$ , sample until convergence :
  1.  $\tilde{\alpha}_k \sim \tilde{\alpha} | \mathbf{z}, \tilde{m}_{k-1}, \tilde{\sigma}_{k-1}^2, C_{k-1}$  (Gaussian),
  2.  $C_k \sim C | \mathbf{z}, \tilde{\alpha}_k$  (Gaussian),
  3.  $\tilde{\sigma}_k^2 \sim \tilde{\sigma}^2 | \tilde{m}_k, \tilde{\alpha}_k$  (inverse-gamma),
  4.  $\tilde{m}_k \sim \tilde{m} | \tilde{\sigma}_k^2, \tilde{\alpha}_k$  (Gaussian),



The Sobol indice for Model  $A_j$  and experiment  $i$  quantifies the fraction of the output variance that is due to  $A_j$ .

$$S_j(\mathbf{x}_i) = \frac{\mathbb{V}[z_i] - \mathbb{E}[\mathbb{V}[z_i|A_j]]}{\mathbb{V}[z_i]} = \frac{\mathbb{V}[\mathbb{E}[z_i|A_j]]}{\mathbb{V}[z_i]} = \frac{\sigma_j^2 \times h_i(j)^2}{h_i^T \text{diag}(\sigma^2) h_i + \sigma_{\epsilon_i}^2}$$

Based on the marginal likelihood  $[\mathbf{z}|m, \sigma^2]$  after integrating with respect to the missing samples, we can prove that the Fisher information matrix is written as

$$I_n(m, \sigma^2) = \begin{pmatrix} I_n(m) & 0 \\ 0 & I_n(\sigma^2) \end{pmatrix}$$

where

$$I_n(m)_{j,k} = \sum_{i=1}^n \frac{h_i(j)h_i(k)}{h_i^T \text{diag}(\sigma^2) h_i + \sigma_{\epsilon_i}^2} \quad 1 \leq j, k \leq p$$

Therefore, we can get

$$I_n(m_j) = \frac{n\bar{S}_j}{\sigma_j^2}$$

and

$$I_n(\sigma^2)_{j,k} = \sum_{i=1}^n \frac{0.5 \times h_i^2(j)h_i^2(k)}{h_i^T \text{diag}(\sigma^2) h_i + \sigma_{\epsilon_i}^2} \quad 1 \leq j, k \leq p$$

and

$$I_n(\sigma_j^2) = \frac{nS_j^2}{2\sigma_j^4}$$

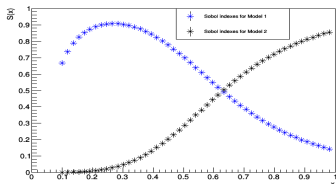
- The smaller the Sobol indice  $S_\Lambda$ , the less accurate the estimates (Celeux et al., 2010):
  - Bayesian counterpart?
    - studying the role of the prior in terms of size of credible regions.
- Well-posedness principles in inverse UQ:
  - in the Hadamard sense (condition number as low as possible)
  - in the Sobol sense:  $S_\Lambda > S_\epsilon$  (i.e. the input contribution to the randomness of  $\mathbf{Z}$  is larger than that of the noise)
  - in the entropy sense, in the Fisher sense (Bousquet and Blazère, 2016).
- In real inverse UQ problems, the Sobol indices are unknown
  - the matrix  $H$  can provide a local sensitivity measure

---

Synthetic example:  $x_i \in [0.1, 1]$ ,  $\alpha = (\alpha_1, \alpha_2)$ ,  $n = 50$

- $z_i = x_i \alpha_{1,i} + 1.6 \times x_i^3 \alpha_{2,i} + \epsilon_i$ 
  - $\alpha_{1,i} \sim \mathcal{N}(2, 0.02^2)$  and  $\alpha_{2,i} \sim \mathcal{N}(2, 0.05^2)$
  - $\epsilon_i \sim \mathcal{N}(0, 0.01^2)$

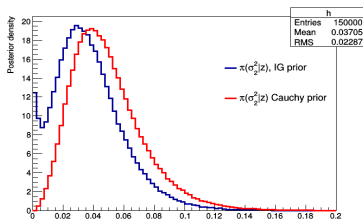
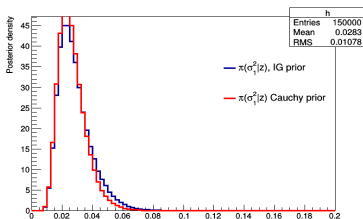
# Relation between inverse UQ and sensitivity analysis



- Sobol indices  $S(x_i)$  against  $x \in [0.1, 1]$
- In averaging over  $x \in [0.1, 1]$ , Model 1 gets higher Sobol indices than Model 2 :
  - $\bar{S}_1 = 0.57$ ,  $\bar{S}_1 = 0.39$  and  $\bar{S}_\epsilon = 0.04$

- Comparison of marginal posterior distributions  $[\sigma_j^2 | \mathbf{z}]$  according to the prior distribution in attempting to make a default Bayesian estimation:

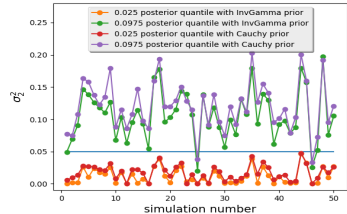
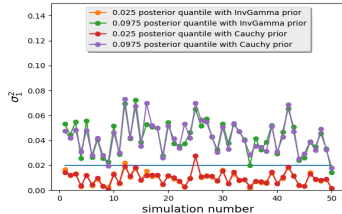
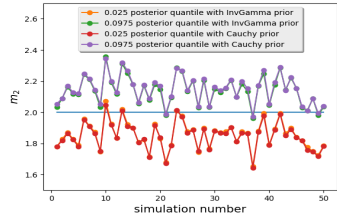
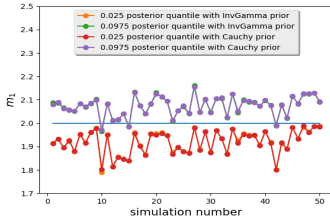
- $\mathcal{IG}(\epsilon, \epsilon)$  with  $\epsilon = 10^{-3}$  for  $\sigma_j^2$  vs half-Cauchy with  $S = 20$  for  $\sigma_j$  ( $j = 1, 2$ )

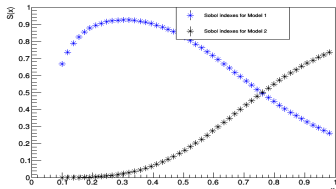


# Impact of the prior: $\text{IG}(\epsilon, \epsilon)$ for $\sigma^2$ vs half-Cauchy for $\sigma$

## ■ Comparison being done over 50 simulated data set:

- credible intervals at 95% are calculated in two cases:  $\mathcal{IG}(0.001, 0.001)$  vs half-Cauchy with  $S = 20$



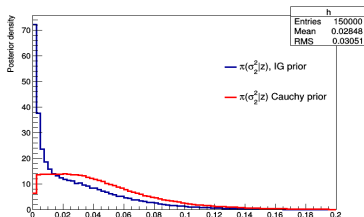
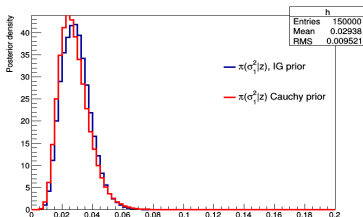


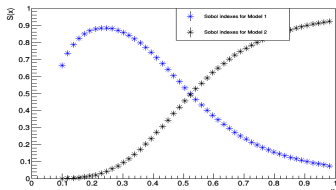
Synthetic example:  $x_i \in [0.1, 1]$ ,  
 $\alpha = (\alpha_1, \alpha_2)$ ,  $n = 50$

- $z_i = x_i \alpha_{1,i} + 1.1 \times x_i^3 \alpha_{2,i} + \epsilon_i$
- $\bar{S}_1 = 0.67$ ,  $\bar{S}_1 = 0.28$  and  $\bar{S}_\epsilon = 0.04$

## ■ Comparison of marginal posterior distributions $[\sigma_j^2 | \mathbf{z}]$

- $\mathcal{IG}(\epsilon, \epsilon)$  with  $\epsilon = 10^{-3}$  for  $\sigma_i^2$  vs half-Cauchy with  $S = 20$  for  $\sigma_j$  ( $j = 1, 2$ )



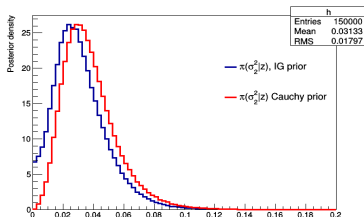
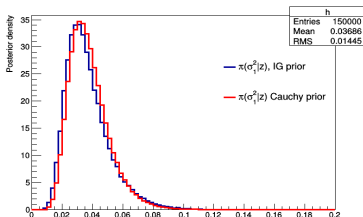


Synthetic example:  $x_i \in [0.1, 1]$ ,  
 $\alpha = (\alpha_1, \alpha_2)$ ,  $n = 50$

- $z_i = x_i \alpha_{1,i} + \mathbf{2.3} \times x_i^3 \alpha_{2,i} + \epsilon_i$
- $\bar{S}_1 = 0.47$ ,  $\bar{S}_1 = 0.49$  and  $\bar{S}_\epsilon = 0.04$

## ■ Comparison of marginal posterior distributions $[\sigma_j^2 | \mathbf{z}]$

- $\mathcal{IG}(\epsilon, \epsilon)$  with  $\epsilon = 10^{-3}$  for  $\sigma_j^2$  vs half-Cauchy with  $S = 20$  for  $\sigma_j$  ( $i = 1, 2$ )



## STEPS FOR BAYESIAN CIRCE:

1. Make linear approximation at  $\alpha_{nom} = \log \lambda_{nom}$  (begin at the nominal  $\alpha_{nom} = \mathbf{0}_p$ )
2. Sample the joint posterior distribution  $m, \sigma^2 | \mathbf{z}$ 
  - if the MAP for  $m$  is close to  $\alpha_0$ , then go to the next step
  - else, go back to Step 1 (Iterative Bayesian Circe)
3. Calculate the marginal distribution of  $A$  :

$$[A] = \int [A|m, \sigma^2][m, \sigma^2 | \mathbf{z}] dm d\sigma^2$$

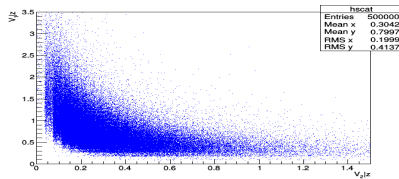
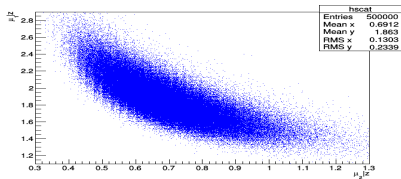
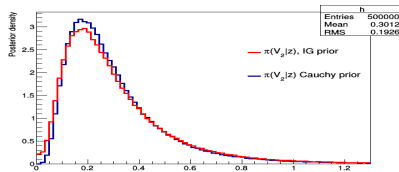
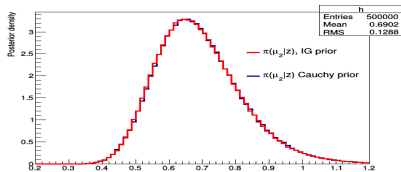
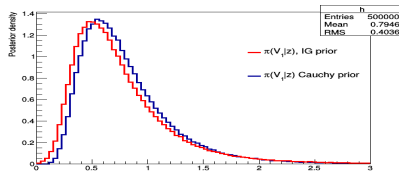
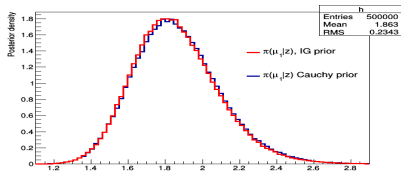
4. Check the validity of the linear assumption on  $\text{IF}_{0.95}(A_j)$  for  $1 \leq j \leq p$ ,
5. Deduce  $\text{IF}_{0.95}(\Lambda_j)$  for  $1 \leq j \leq p$ .

---

## APPLICATION TO THE CONDENSATION MODELS

- 50 tests with two output values: condensation flow rate and temperature
  - ⇒  $n = 100$  physical measurements. Two models are considered:
    - Model  $\Lambda_1$  (flow rate on the free surface in area  $B$ )
    - Model  $\Lambda_2$  (flow rate due to the turbulent mixing in area  $C$ )

# Results (Gibbs implemented with the ROOT library)





Non linear generalization

Instead of linearizing the computer code, we aim to tackle the exact situation where  $Y(\cdot)$  is non-linear with respect to  $\alpha$  :

- $\tilde{\alpha}_k \sim \tilde{\alpha} | \mathbf{z}, \tilde{m}_{k-1}, \tilde{\sigma}_{k-1}^2, C_{k-1}$  is no longer Gaussian  $\implies$  MH sampling  $\implies$  **MH within Gibbs algorithm**
- $Y(\cdot)$  is thermal-hydraulic system code, moderately time-consuming (several minutes per simulation)  
 $\implies$  several weeks for a converged Gibbs sampler, along with possible failed simulations.
- Emulator is needed such as **Gaussian process (GP)**, neural networks. GP interpolates the learning simulations, which is expected for deterministic ones:  
 $\implies \tilde{\alpha}_k \sim \tilde{\alpha} | \mathbf{z}, \tilde{m}_{k-1}, \tilde{\sigma}_{k-1}^2, C_{k-1}$  is based on both mean and variance of the GP emulator.
- How to control the gap between the GP-based posterior distribution and the actual one?
  - see Barbillon (2017) in the context of mixed models from a classic point of view (SAEM algorithm instead of MH-within Gibbs).

Some questions/future works

- How to specify priors for scale parameters in hierarchical models when an objective Bayesian estimation is expected ?
  - Should we specify a prior for the scale  $S$  of the half-Cauchy prior?
  - How to measure how strong the estimation is data-dominated?
  - Studying the frequentist properties of credible intervals obtained from various priors proposed in the literature including the half-Cauchy.
- Statistical modeling to carry out in future works:
  - Estimating the experimental variances  $\sigma_{\epsilon_i}^2$  when they are unknown, promoting the multidimensional version, taking into account a model  $\Lambda_k$  that is already known,
  - Assuming a functional multiplier coefficient  $\Lambda(x)$  as a log-Gaussian process (functional Bayesian CIRCE).
- Convergence diagnostics to implement for future users in CEA (I hope so !).

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