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Inverse uncertainty quantification applied to thermal-hydraulic simulations

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Outline

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 ?
Uncertainties at all stages

CONCEPTION OF CORRELATIONS

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

\[ C_{\text{nom}}(x, \theta) \]

where \( x \) 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
    \[ \rightarrow \text{inverse UQ process} \]
The CIRCE method
**Main Assumptions**

- Model uncertainty is multiplicative:
  \[ C_\Lambda(x) = \Lambda \times C_{nom}(x) \]

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

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

**STATISTICAL MODELING**

- \( z_i \in \mathbb{R} \) the QoI experimentally measured at \( x_i \in \mathbb{R}^m \)
- \( Y(.) \) the CATHARE 2 code (used as a black-box function)
- For \( i \in [1; n] \), we assume that

\[
\begin{align*}
  z_i &= Y(C_{\lambda_1,i}(x_i), \ldots, C_{\lambda_p,i}(x_i)) + \epsilon_i \\
  &= Y(\lambda_1,i,\ldots,\lambda_p,i)(x_i) + \epsilon_i
\end{align*}
\]

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

The CIRCE method consists in estimating \( m_j \) and \( \sigma_j^2 \) for \( j \in [1; p] \).
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 $C_{\lambda_1}(x_i)$ (area B) and $C_{\lambda_2}(x_i)$ (area C)

$$Q_i = Y_{\lambda_1,i,\lambda_2,i}(x_i) + \epsilon_i$$

where $x_i$ includes injection pressure, injection temperature, water height in the cold leg, etc.
OTHER ASSUMPTIONS UNDERLYING CIRCE:

- The factors are not correlated each other: $\text{Cov}(\Lambda_j, \Lambda_k) = 0 ; 1 \leq j \neq k \leq p$,
- 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 $0_p = \log 1_p$
   - $z_i - Y_i^{nom} = h_i^T (\alpha_i - \alpha_{nom}) + \epsilon_i$ with $\alpha_i := \log \lambda_i$
   - Identifiability: $\text{rank}(H) = p$ where $H = [h_1, \cdots, h_n]^T \in \mathcal{M}_{np}$.

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

Notations:

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

Statistical model

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

Posterior distribution

- Bayes formula gives \( [m, \sigma^2 | \mathbf{z}, \mathbf{\alpha}] \propto [\mathbf{z}, \mathbf{\alpha} | \sigma^2, m][m, \sigma^2] \)
  - Likelihood: \( \mathbf{z} | \mathbf{\alpha}, \sigma^2, m \sim \otimes_{i=1}^{n} \mathcal{N}(h_i^T \alpha_i, R_i) \),
  - 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).
**Prior distributions**

**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 \(i \in [1; n]\), with \(\tilde{\alpha}_i = C\alpha_i\)
  - Priors: \(C \sim \mathcal{N}(m_C, 1)\) and \(\sigma^2_{\tilde{\alpha}} \sim \mathcal{IG}(0.5 \times \nu, S)\)
  - 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 \(S \rightarrow +\infty\))
  

\[
[\sigma] \propto \frac{1}{\sigma^2 + S}
\]
**MCMC algorithms in the standard model**

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

By following the hierarchical structure \([m, \sigma^2, \alpha | z] = [m, \sigma^2 | \alpha, z][\alpha | z]\)

- Start with a first sample \((m_0, \sigma^2_0)\)
- In a loop \(k \geq 1\), sample until convergence:
  1. \(\alpha_k \sim \alpha | z, m_{k-1}, \sigma^2_{k-1}\) (Gaussian),
  2. \(m_k, \sigma^2_k \sim m, \sigma^2 | \alpha_k, z\) (Gaussian-inverse-gamma).

**GIBBS SAMPLING**

Based on the full conditional posterior distributions

- Start with a first sample \((m_0, \sigma^2_0)\)
- In a loop for \(k \geq 1\), sample until convergence:
  1. \(\alpha_k \sim \alpha | z, m_{k-1}, \sigma^2_{k-1}\) (Gaussian),
  2. \(m_k \sim m | \sigma^2_k, \alpha_k, z\) (Gaussian),
  2. \(\sigma^2_k \sim \sigma^2 | b_k, \alpha_k, z\) (inverse-gamma),
MCMC algorithms in the augmented model

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

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

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

GIBBS SAMPLING

Based on the full conditional posterior distributions:

- Start with a first sample \((\tilde{m}_0, \tilde{\sigma}^2_0, C_0)\)
- In a loop for \(k \geq 1\), sample until convergence:
  1. \(\tilde{\alpha}_k \sim \tilde{\alpha} | z, \tilde{m}_{k-1}, \tilde{\sigma}^2_{k-1}, C_{k-1}\) (Gaussian),
  2. \(C_k \sim C | z, \tilde{\alpha}_k\) (Gaussian),
  3. \(\tilde{\sigma}^2_k \sim \tilde{\sigma}^2 | \tilde{m}_k, \tilde{\alpha}_k\) (inverse-gamma),
  4. \(\tilde{m}_k \sim \tilde{m} | \tilde{\sigma}^2_k, \tilde{\alpha}_k\) (Gaussian),
The Sobol indice for Model $A_j$ and experiment $i$ quantifies the fraction of the output variance that is due to $A_j$.

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

Based on the marginal likelihood $[z|m, \sigma^2]$ 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

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

and

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

Therefore, we can get

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

and

$$I_n(\sigma_j^2) = \frac{n S_j^2}{2\sigma_j^4}$$
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 $Z$ 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 $\bar{S}_e = 0.04$

Comparison of marginal posterior distributions $[\sigma^2_j | z]$ according to the prior distribution in attempting to make a default Bayesian estimation:
- $\mathcal{IG} (\epsilon, \epsilon)$ with $\epsilon = 10^{-3}$ for $\sigma^2_j$ vs half-Cauchy with $S = 20$ for $\sigma_j$ ($j = 1, 2$)
Comparison being done over 50 simulated data set:

- credible intervals at 95% are calculated in two cases: $IG(0.001, 0.001)$ vs half-Cauchy with $S = 20$
A worse case

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 $[\sigma_j^2 | z]$

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

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

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

**Comparison of marginal posterior distributions \([\sigma^2_j | z]\)**

- \( IG(\epsilon, \epsilon) \) with \( \epsilon = 10^{-3} \) for \( \sigma^2_j \) vs half-Cauchy with \( S = 20 \) for \( \sigma_j \) (\( i = 1, 2 \))
Application to the condensation tests

**Steps for Bayesian Circe:**

1. Make linear approximation at $\alpha_{nom} = \log \lambda_{nom}$ (begin at the nominal $\alpha_{nom} = 0$)

2. Sample the joint posterior distribution $m, \sigma^2 | z$
   - 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 $A$:

   $$ [A] = \int [A|m, \sigma^2] [m, \sigma^2 | z] dmd\sigma^2 $$

4. Check the validity of the linear assumption on $IF_{0.95}(A_j)$ for $1 \leq j \leq p$.

5. Deduce $IF_{0.95}(\Lambda_j)$ for $1 \leq j \leq p$.

**Application to the Condensation Models**

- 50 tests with two output values: condensation flow rate and temperature.
  $\iff n = 100$ 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)

Inverse UQ applied to TH simulations

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Non linear generalization
Non linear setting

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

- $\tilde{\alpha}_k \sim \tilde{\alpha}|z, \tilde{m}_k, \tilde{\sigma}^2_k, C_k$ is no longer Gaussian $\implies$ MH sampling $\implies$ MH within Gibbs algorithm

- $Y(.)$ 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:
  $\implies$ $\tilde{\alpha}_k \sim \tilde{\alpha}|z, \tilde{m}_k, \tilde{\sigma}^2_k, C_k$ 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
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 $\sigma^2_{\epsilon_i}$ when they are unknown, promoting the multidimensional version, taking into account a model $\Lambda_{k_i}$ 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!).


