DE LA RECHERCHE À L'INDUSTRIE

Inverse uncertainty quantification of input model parameters in thermal-hydraulic simulation

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Workshop on calibration of numerical code

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Prelude

Thank you to my colleagues and co-authors for the great collaboration!

Summary

1. Context and motivations
2. The CIRCE method
3. Multi-group CIRCE
4. Related works

Context and motivations

Thermal-hydraulic simulation in the nuclear field

- Needed to simulate power plants (innovative or in operation) as well as for safety analyses of hypothetical accidental scenarios.
- Simulations run by **Best Estimate** computer codes with a great effort to V&V (ex: the CATHARE code in CEA).
- Based on balance equations (mass, momentum and energy) which require **closure models** due to time and space averaging.
- Example: the energy equation applied to a control volume:

$$\rho \overbrace{\frac{\partial I}{\partial t}}^{(1)} = - \overbrace{\text{grad}(\dot{\mathbf{q}}'')}^{(2)} + \overbrace{\dot{q}'''}^{(3)} + \overbrace{\frac{\partial P}{\partial t}}^{(4)} + \overbrace{\phi}^{(5)}$$

(1) variation in time of enthalpy, **(2) and (3) are heat fluxes which should be modeled by (semi)-empirical models**, (4) variation in time of the pressure, (5) dissipation function.

From modeling to simulation

"Nominal" closure models:

- Established by means of both expertise and well-chosen experimental data, and denoted by

$$M_{nom}(\mathbf{x}),$$

with $\mathbf{x}$ being thermal-hydraulic and design variables,

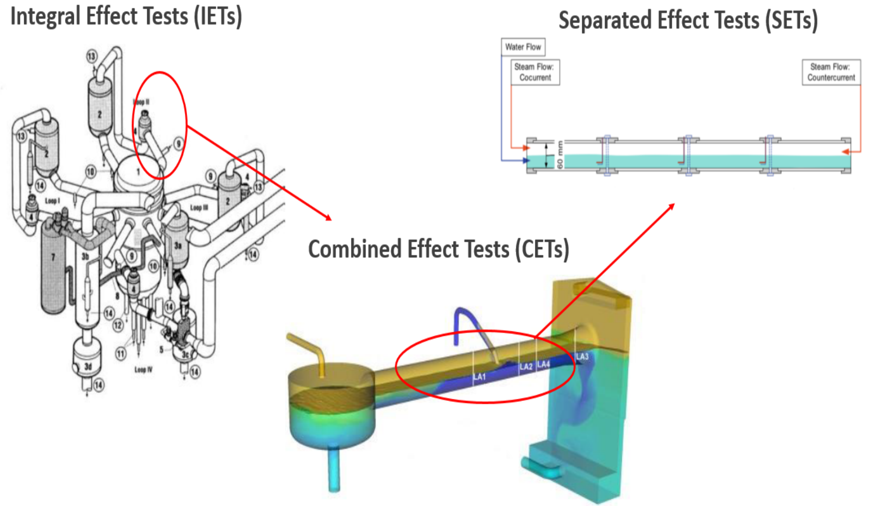
- Experimental uncertainty on $\mathbf{x}$ may occur but is often neglected in practice.

Simulations:

i) Implemented from appropriate closure models $\Longrightarrow$ numerical uncertainties to check (verification task).

ii) Comparisons between the simulations and corresponding experimental data (validation task).

iii) Assessment of model uncertainty from the discrepancy between the two $\Longrightarrow$ **IUQ (inverse uncertainty quantification).**


Integral Effect Tests (IETs)
Separated Effect Tests (SETs)
Combined Effect Tests (CETs)
Water Flow
Steam Flow: Cocurrent
Steam Flow: Countercurrent
60 mm
Loop I
Loop II
Loop III
Loop IV
LA1
LA2
LA4
LA3

The CIRCE method

CIRCE $=$ *Calcul des Incertitudes Relatives aux Corrélations Élémentaires* (De Crécy and Bazin, 2001).

Main assumptions:

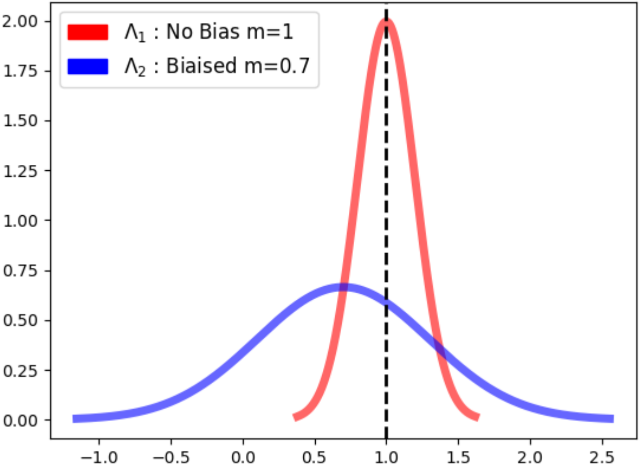
- Model uncertainty is multiplicative:

$$M_\lambda(\mathbf{x}) = \lambda \times M_{nom}(\mathbf{x})$$

- λ is modeled as a probability distribution $\Longrightarrow M_\lambda$ is aleatory,
- λ is Gaussian $\mathcal{N}(m, \sigma^2)$,
- Model uncertainty is known as "unbiased" if $m = 1$.

We wish that the bias, equal to $1 - \hat{m}$, is as small as possible.

Biased versus unbiased distributions



CIRCE is an inverse problem

Probabilistic link between the experimental data and simulations:

- $y_i \in \mathbb{R}$ the experimental QoI at $\mathbf{x}_i$ (for $i \in [\![1; n]\!]$),
- G the CATHARE code (used as a black-box),
- We assume that

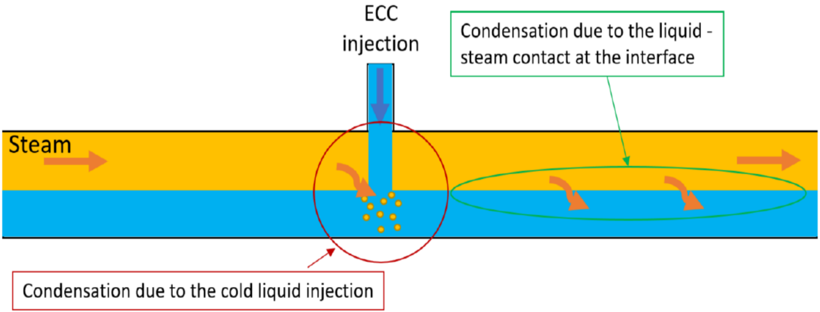
$$\begin{aligned} y_i &= G(\overbrace{M_{\lambda_{1,i}}(\mathbf{x}_i), \cdots, M_{\lambda_{p,i}}(\mathbf{x}_i)}^{Aleatory\ closure\ models}) + \epsilon_i \\ &= G_{\lambda_i}(\mathbf{x}_i) + \epsilon_i \end{aligned}$$

where

- $\lambda_i = (\lambda_{1,i}, \cdots, \lambda_{p,i})^T \in \mathbb{R}^p$ with $\lambda_{j,i} \sim \mathcal{N}(m_j, \sigma_j^2)$, $j \in [\![1; p]\!]$.
- $\epsilon_i \sim \mathcal{N}(0, \sigma_{\epsilon_i}^2)$.

The CIRCE method jointly estimates all the m_j and σ_j^2 (SETs: $p = 1$, CETs: $p \geq 2$).

Ex : Emergency Core Cooling injection (Cocci, 2022)



This is a CET: $p = 2$ condensation phenomena, modeled respectively by $M_{\lambda_1}(.)$ and $M_{\lambda_2}(.)$, take place at the same time.

CIRCE consists of three main steps:

1) Linearization of the simulations in λ at the nominal model, i.e. $\lambda^\star = \mathbf{1}_p$

$$y_i - G_{\lambda^\star}(\mathbf{x}_i) = h_i^T(\lambda_i - \lambda^\star) + \epsilon_i, \quad i \in [\![1; n]\!].$$

2) Joint computation of **Maximum Likelihood estimates** $(\hat{m}_j, \hat{\sigma}_j^2)$ if $H = [h_1, \cdots, h_n]^T \in \mathcal{M}_{n,p}(\mathbb{R})$ is full rank.

3) Confirmation of the results through a posterior inspection of both linearity and normality assumptions.

In this presentation, we are focusing on the second step!

Notations used in the sequel

- Mean parameters $m := (m_1, \cdots, m_p)^T \in \mathbb{R}^p$,
- Variance parameters $\sigma^2 := (\sigma_1^2, \cdots, \sigma_p^2)^T \in \mathbb{R}^p$,
- Shifted observed data $Y := (y_1 - G_{\lambda^\star}(\mathbf{x}_1), \cdots, y_n - G_{\lambda^\star}(\mathbf{x}_n))^T \in \mathbb{R}^n$,
- Shifted latent data $\lambda := (\lambda_1 - \lambda^\star, \cdots, \lambda_n - \lambda^\star)^T \in \mathcal{M}_{n,p}(\mathbb{R})$,
- Shifted complete data $Z := \{Y, \lambda\}$.

Complete and marginal likelihood

- Complete likelihood: $L(Z|m,\sigma^2) = \overbrace{L(Y|\lambda,m,\sigma^2)}^{Gaussian}\overbrace{L(\lambda|m,\sigma^2)}^{Gaussian}$ with

$$L(Y|\lambda,m,\sigma^2) \propto \prod_{i=1}^{n} \exp\Big(-\frac{1}{2}\frac{\big(Y_i - h_i^T\lambda_i\big)^2}{\sigma_{\epsilon_i}^2}\Big)$$

and

$$L(\lambda|m,\sigma^2) \propto \prod_{i=1}^{n} |\text{diag}(\sigma^2)|^{-1/2} \exp\Big(-\frac{1}{2}(\lambda_i - m)^T\text{diag}(\sigma^2)^{-1}(\lambda_i - m)\Big).$$

- Marginal likelihood: integrating over λ leads to the likelihood of the observed data only, still Gaussian:

$$L(Y|m,\sigma^2) \propto \prod_{i=1}^{n}(h_i^T\text{diag}(\sigma^2)h_i+\sigma_{\epsilon_i}^2)^{-1/2} \exp\Big(-\frac{1}{2}\frac{(Y_i - h_i^T m)^2}{h_i^T\text{diag}(\sigma^2)h_i + \sigma_{\epsilon_i}^2}\Big).$$

The ECME algorithm for MLE

ECME $=$ *Expectation-Conditional Maximization Either* (Celeux et al., 2010)

1. Step of Expectation (E): calculation of

$$Q((m,\sigma^2),(m^k,\sigma^{2,k})) = \mathbb{E}_\lambda[l(Z|m,\sigma^2)|Y,m^k,\sigma^{2,k}].$$

   The expectation is taken with respect to the distribution of λ conditional on $(Y, m^k, \sigma^{2,k})$.

2. Steps of Conditional Maximization (CM):

   - CM1: $\sigma^{2,k+1} = \underset{\sigma^2}{\operatorname{argmax}}\, Q((m,\sigma^2),(m^k,\sigma^{2,k}))$,
   - CM2: $m^{k+1} = \underset{m}{\operatorname{argmax}}\, l(Y|m^k,\sigma^{2,k+1})$.

- CM1 and CM2 have **analytic expressions** as functions of $(m^k, \sigma^{2,k})$.
- Starting from a first sample (m_0, σ_0^2), the convergence of the ECME algorithm is **faster than that of EM.**

CIRCE using CETs in practice

CIRCE on CETs

- $p \geq 2$ factors estimated jointly from Y, often in a small data context $(50 \leq n \leq 200)$,
- If $H_{\star 1} >> H_{\star 2}$ (case $p = 2$), then the estimators $(\hat{m_2}, \hat{\sigma}_2^2)$ and $(\hat{m_1}, \hat{\sigma}_1^2)$ may be respectively inaccurate and degraded.

Multi-stage CIRCE: (Cocci et al., 2022)

- CETs can still be used, but to estimate only the dominant factor, say λ_1, while neglecting the other ones,
- If being known, the uncertainty of the other factors λ_j $(2 \leq j \leq p)$ adds up to the experimental uncertainty (case $p = 2$ below):

$$Y_i = h_{i1}\lambda_{1,i} + \epsilon_i \quad \text{with} \quad \epsilon_i \sim \mathcal{N}\left(h_{i2}m_2, h_{i2}^2\sigma_2^2 + \sigma_{\epsilon_i}^2\right).$$
$$\Longleftrightarrow$$
$$Y_i - h_{12}m_2 = h_{i1}\lambda_{1,i} + \epsilon_i \quad \text{with} \quad \epsilon_i \sim \mathcal{N}\left(0, h_{i2}^2\sigma_2^2 + \sigma_{\epsilon_i}^2\right).$$

Multi-group CIRCE

Multi-group CIRCE (Damblin et al., 2023)

Motivation:

The model uncertainty may not be the same across the whole set of experimental tests Y. How to statistically check on it ?

- Y is now made up of s groups of different experimental setups:

$$Y := (Y_1, \cdots, Y_s, \cdots, Y_l)^T \in \mathbb{R}^n \quad ; \quad 1 \leq s \leq l$$

- A variance parameter σ_s^2 is estimated for each group jointly to a mean parameter m common to every group.
- For example, Y_s may have a specific geometry or thermal-hydraulic input range.
- Let i_s denote the last index of the s-th group. Then,

$$i_{s-1} + 1 \leq i \leq i_s \implies \lambda_i \sim \mathcal{N}(m, \sigma_s^2)$$

Multi-group complete likelihood:

$$L(Z|m,\sigma_1^2,\cdots,\sigma_l^2) = L(Y|\lambda,m,\sigma_1^2,\cdots,\sigma_l^2)L(\lambda|m,\sigma_1^2,\cdots,\sigma_l^2)$$

with

$$L(\lambda|m,\sigma_1^2,\cdots,\sigma_l^2) \propto \prod_{s=1}^{l}\prod_{i=i_{s-1}+1}^{i_s}\Big[|\text{diag}(\sigma_s^2)|^{-1/2} \exp\Big(-\frac{1}{2}(\lambda_i-m)^T\text{diag}(\sigma_s^2)^{-1}(\lambda_i-m)\Big)\Big].$$

Both E. and CM. steps of the multi-group ECME are **still analytic**, and thus the MLE is readily computable.

The Wald test in the multi-group CIRCE

We aim to evaluate the degree of statistical evidence that the variances of the groups are different to one another.

- Null hypothesis: $\mathcal{H}_0 \ : \ \sigma_s^2 - \sigma_{s'}^2 = 0, \quad 1 \leq s \neq s' \leq l.$
- The **Wald's statistic** is written as:

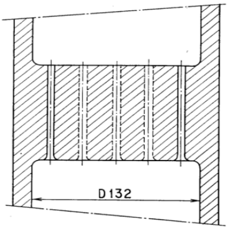
$$W = \frac{(\hat{\sigma}_s^2 - \hat{\sigma}_{s'}^2)^2}{\mathbb{V}[\hat{\sigma}_s^2] + \mathbb{V}[\hat{\sigma}_{s'}^2] - 2\text{Cov}(\hat{\sigma}_s^2, \hat{\sigma}_{s'}^2)} \sim \chi^2(1) \ \text{ under } \ \mathcal{H}_0,$$

  with $\chi^2(1)$ denoting the chi-square distribution with one degree of freedom.

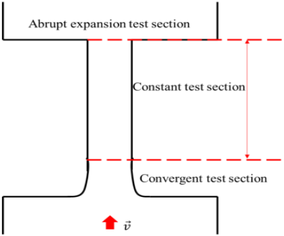
- The test can be applied to each pair of indexes $1 \leq s \neq s' \leq l$.

Application to the critical mass flow

- Discharge of coolant flow due to pressure drop at the break.
- The mass flow rate reaches a maximum value called **critical mass flow** (or chocked flow).
- Several types of SETs for this phenomenon, including BETHSY Nozzle 2 (B2) and BETHSY Nozzle 6 (B6).



a) BETHSY 2"



b) BETHSY 6"

Application to the critical mass flow

Is the uncertainty influenced by the geometry?

- $p = 1 : M_{nom}$ is the so-called flashing model,
- $Y = Y_{B2} \cup Y_{B6}$ with $n_{B2} = 25$ and $n_{B6} = 24$,
- Simulations run with the CATHARE code,
- Log-Linearization was more accurate $\Longrightarrow \lambda \sim \mathcal{LN}(m, \sigma^2)$,
- The multi-group ECME gives:

$$\hat{m} = 0.57 \text{ and } (\hat{\sigma}^2_{B2}, \hat{\sigma}^2_{B6}) = (0.31, 0.13).$$

- $W = 3.62$ and $\mathbb{P}[\chi^2(1) \leq 3.84] = 0.95$. The equality of variances is thus not rejected at the 5% level.

Related works

Related works

- Non-linear CIRCE (Barbillon et al., 2011), Bayesian CIRCE (Damblin and Gaillard, 2020).
- Assessment of the **adequacy** of experimental databases through the criteria of representativeness and completeness (Baccou et al., 2019).
- On going-OCDE project, named **ATRIUM**, on the realization of IUQ methods by numerous worldwide participants.
- Scaling issue: do the uncertainties remain valid on IETs or ultimately on an actual power plant?

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