Statistical methodology for uncertainty quantification/propagation for materials

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Works derived by collaboration with:

Riccardo Cocci
Guillaume Damblin
Alberto Ghione
…and in the framework of the OECD/NEA ATRIUM activity

Summary

1. Calibration under uncertainty

The importance of the experimental data

The importance of the physics

The importance of the statistical model

2. Uncertainty of assessed model

The importance of sensitivity analysis

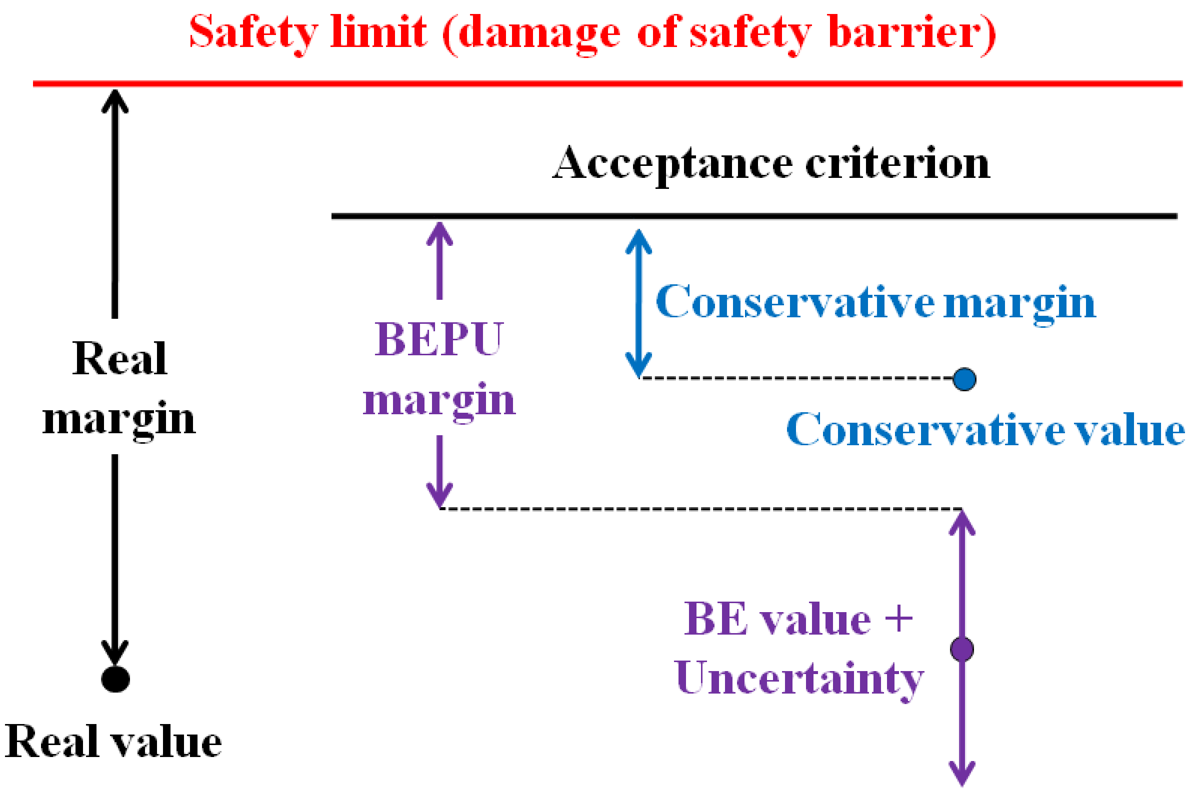
The importance of the statistical model for the quantification

Available methodologies for safety studies

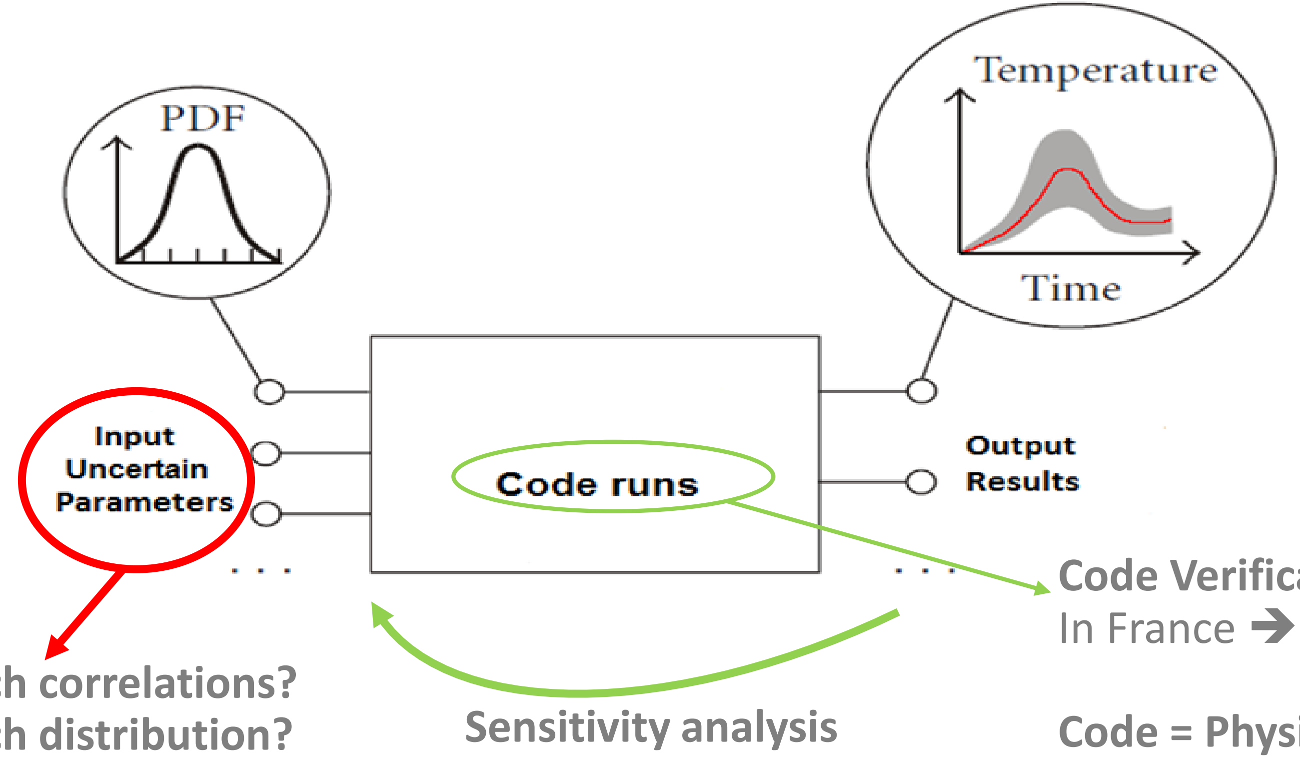
Safety demonstration ➔ a lot of simulations

Conservative method	vs	Best Estimate Plus Uncertanties (BEPU) method
One « penalizing » simulation		« The most realistic simulation» + **Uncertainty quantification**

Conservative margin vs Best-Estimate Plus Uncertainties (BEPU)



Simulations for BEPU methodology



Which correlations?
Which distribution?
Which inlet conditions?

Sensitivity analysis

Code Verification & Validation
In France ➔ Guide ASN n°28

Code = Physical models! ☺

...and in France

Guide n°28

Le présent guide expose les recommandations de l'ASN et de l'IRSN pour ces opérations et ce processus. Il a pour objet de fournir un ensemble cohérent de recommandations dont la mise en œuvre constitue une manière de s'assurer qu'un OCS (Outils de Calcul Scientifique, n.d.l.r) est qualifié selon les attentes de l'ASN. Il a pour ambition de faciliter l'élaboration et l'instruction des dossiers établissant la qualification(*) des OCS en précisant le contenu du dossier à produire par l'exploitant pour sa transmission à l'ASN.

Reconnaissance par l'exploitant qu'un OCS est apte à fournir des résultats utilisables dans le cadre de la **démonstration de sûreté nucléaire**

Awareness via V&V&UQ of the code to reproduce simulations for the the safety studies !!!

V&V&UQ process

Verification

Doing the things right

ensuring that the OCT works as intended (**correct computer and digital implementation, correct digital results**)

Validation

Doing the right things

ensuring that an OCT can satisfactorily simulate the **physical phenomena** in the validation domain

Depending on experimental data !!!

Uncertainty Quantification

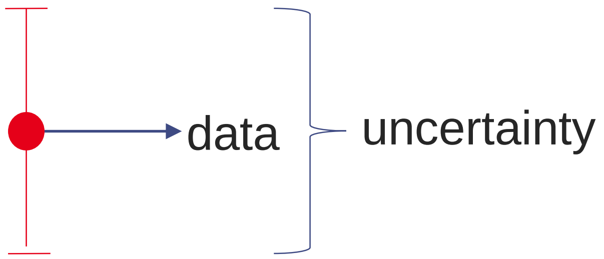
Definition of uncertainty

From *Guide ASN n°28*:

«Range of variation of the result of a measurement or calculation which characterises the possible values and which is likely to contain the true value of the target response under consideration.» (*«Gamme de variation du résultat d'une mesure ou d'un calcul qui caractérise les valeurs possibles et qui contient vraisemblablement la valeur réelle de la réponse cible considérée.»*)

From NEA:

«The uncertainties define the range within which the corresponding data can be reproduced with a probability of 95% at any place and by any appropriate method.»

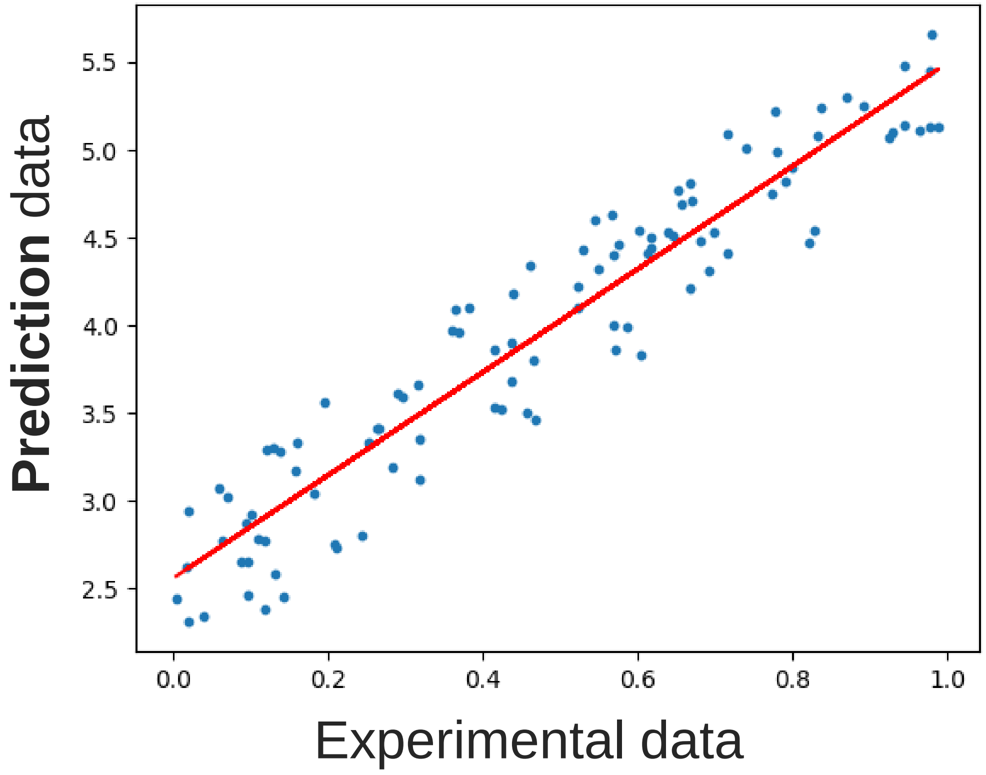


What kind of uncertainties?

- **Experimental uncertainty**, e.g. due to the measurement noise
- **Model and parameter uncertainties**, caused by the incomplete mathematical modelling of the phenomena and the inaccurate calibration of the correlation parameters
- **Code uncertainty**, due to the mathematical approximations and numerical schemes of the code when computing the output value
- **Plant uncertainty**, related to the geometry of the system and its initial and boundary conditions
- **Scaling uncertainty**, due to the use of models developed on scaled experiments to a full-scale reactor
- Representation uncertainty, caused by the **nodalisation** of the systems, i.e. the uncertainty in the physical discretisation
- **User's uncertainty**, related to the modelling choices of the code user

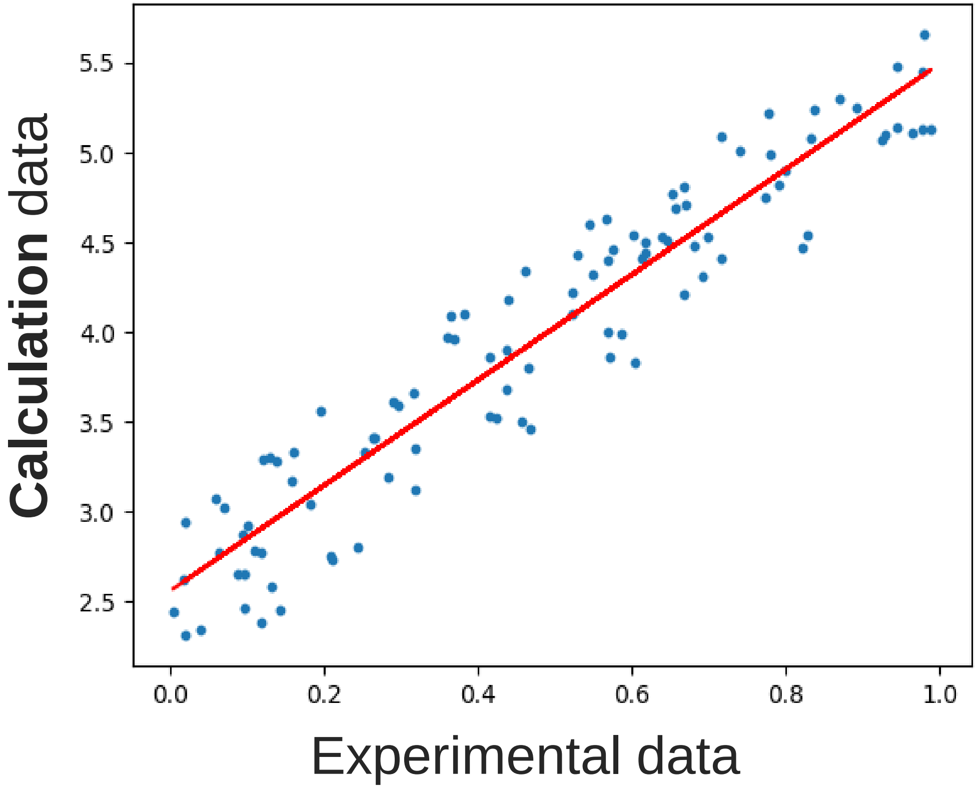
In which cases do we need uncertainty?

Quantification after validation ➔ uncertainty on a **simulated quantity** w.r.t. experiments



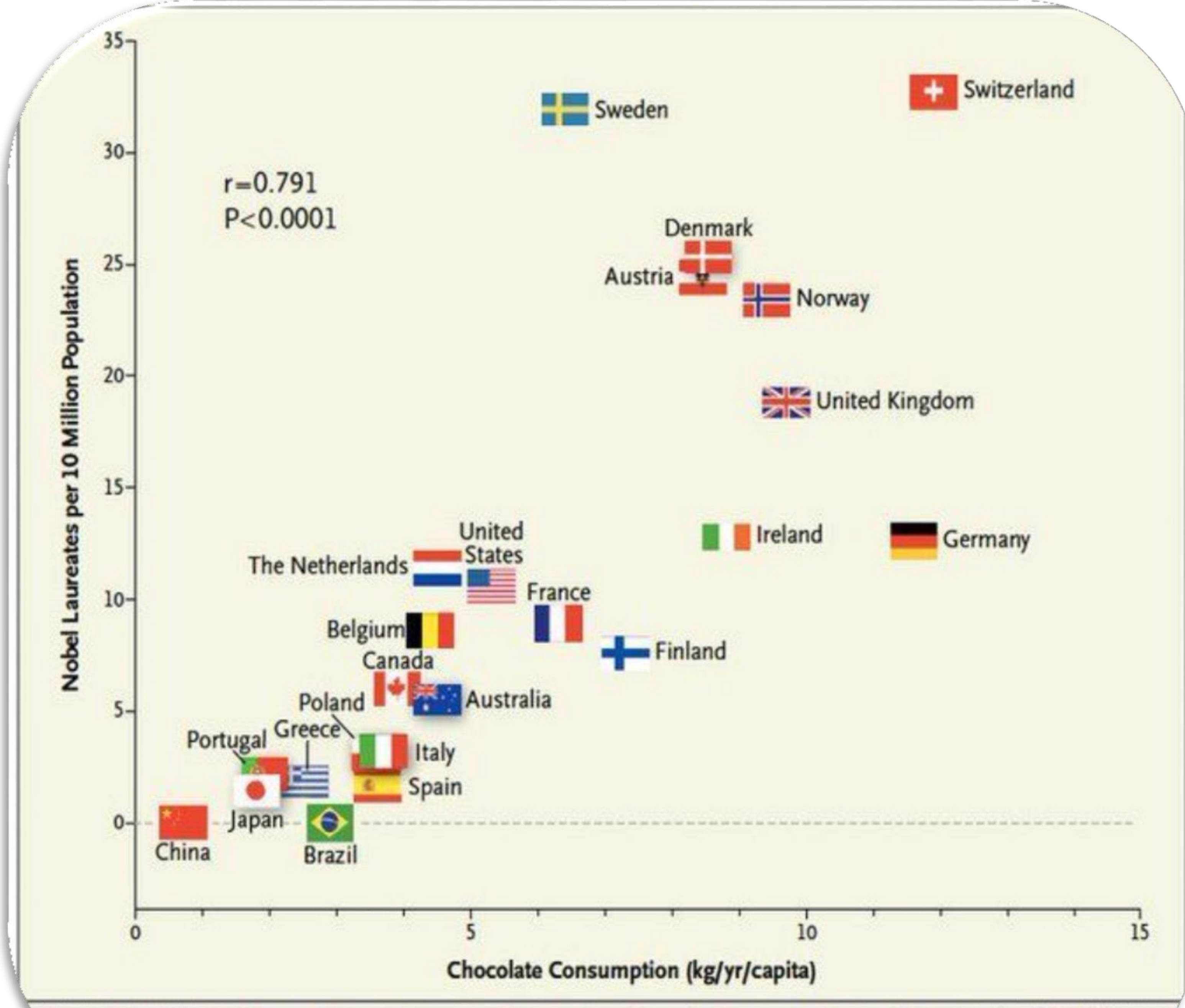
…but before…

Calibration ➔ uncertainty on a assessed quantity via **statistical calibration** w.r.t. experiments



Calibration under uncertainty

A comprehensive Bayesian framework for the development, validation and uncertainty
quantification of thermal-hydraulic models"
R. Cocci, G. Damblin, A. Ghione, L. Sargentini and D. Lucor
Annals of Nuclear Energy 172, 109029, 2022
Available at:
https://www.sciencedirect.com/science/article/pii/S0306454922000640



igure 1. Correlation between Countries' Annual Per Capita Chocolate Consumption and the Number of Nobel
reates per 10 Million Population.

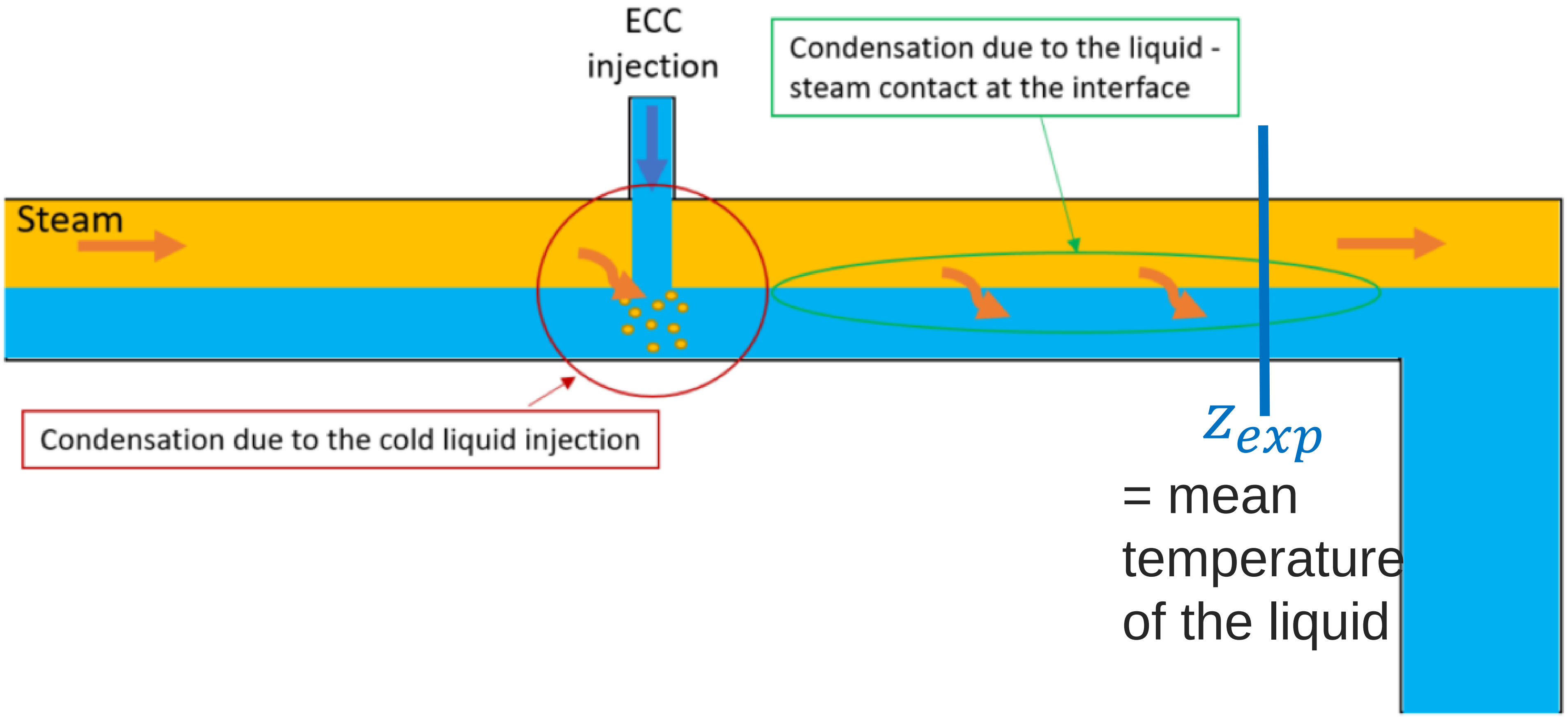
Definition of the statistical problem

$$z_{exp}(x,\theta) = z_{pred}(x,M) + \varepsilon = z_{calc}(x,\theta)\cdot\Lambda(x) + \varepsilon$$

- z_{exp} ➔ experimental Quantity of Interest (QoI)
- x ➔ State variables (e.g. non-dimensional numbers, experimental conditions)
- θ ➔ Parameter
- z_{pred} ➔ predicted/simulated QoI
- M ➔ physical models depending on x, θ
- ε ➔ Experimental error: $\mathcal{N}(\mathbf{0}, \boldsymbol{\sigma}_{exp}^{2})$
- z_{calc} ➔ mathematical QoI, i.e. physical model
- Λ ➔ Model uncertainty ➔ **non reducible** with infinite experimental points

1. The experimental data: how to deal with them?

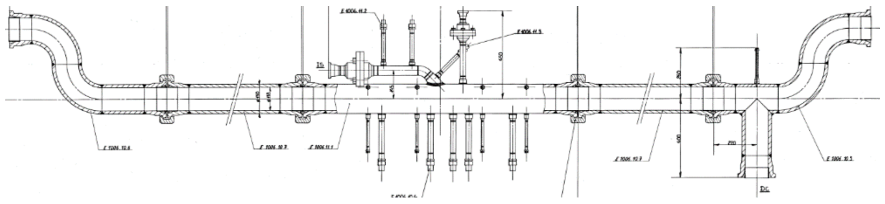
Physical problem: steam jet condensation in a stratified flow

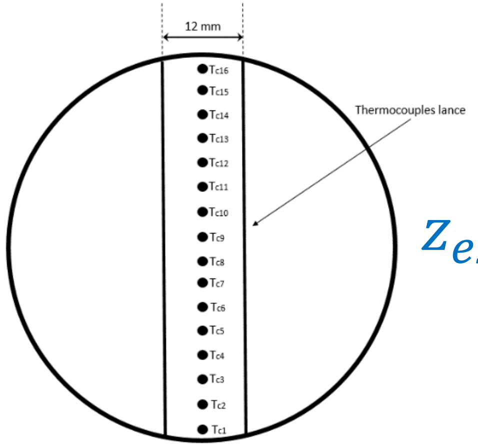


z_{exp} = mean temperature of the liquid

Example of experimental data

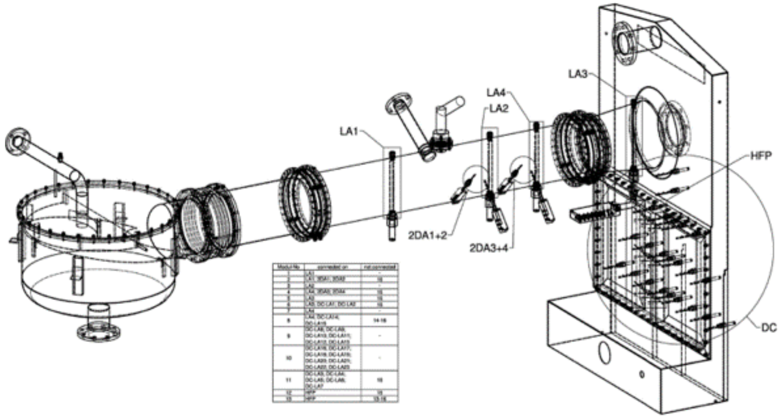
COSI (**C**ombined **E**ffect **T**est)



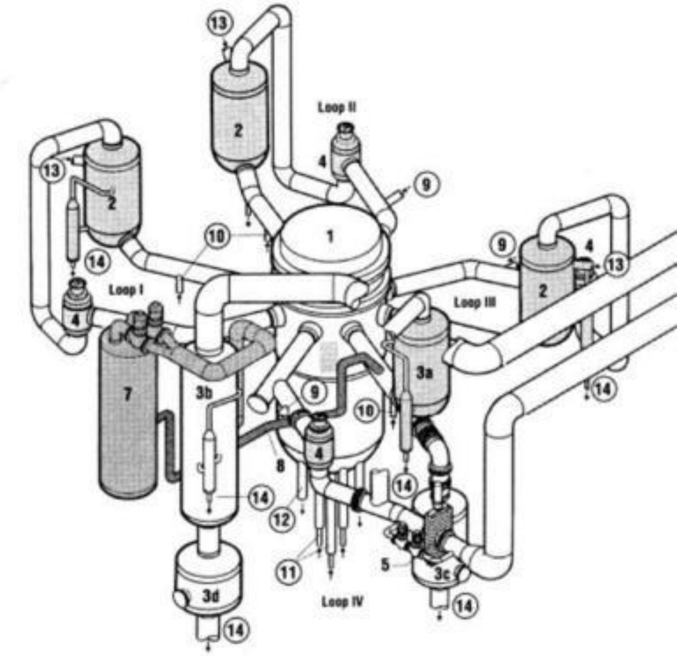


z_{exp} = mean temperature of the liquid

TOPFLOW (**C**ombined **E**ffect **T**est)



UPTF (**I**ntegral **E**ffect **T**est)



Experimental scale

How to define if data are good enough to assess a physical model?

Adequacy = representativeness + completeness

representativeness: ability of each experimental test to provide relevant information for the problem of interest

completeness: ability of a set of experimental tests to cover the physical conditions of the problem of interest

J. Baccou et al.
A systematic approach for the adequacy analysis of a set of experimental databases: Application in the framework of the ATRIUM activity, Nuclear Engineering and Design, Volume 421, 2024, 113035, ISSN 0029-5493, https://doi.org/10.1016/j.nucengdes.2024.113035.

Representativeness and completeness criteria

Generic criteria for adequacy analysis developed in ATRIUM

Representativeness criteria

Criteria	Sub-criteria
C^r_1: Fidelity with the target application facility for the accidental transient of interest	C^r_{1-1}: Fidelity of geometry between experimental and target application facilities
	C^r_{1-2}: Fidelity of thermal-hydraulic conditions between experiment and target application facility
C^r_2: Control of experimental data	(Dedicated list of questions)
C^r_3: Modelling of the physical phenomena for their implementation in the system code	C^r_{3-1}: Capability to cover physical phenomena of interest required for the simulation
	C^r_{3-2}: Separability
	C^r_{3-3}: Capability of the simulation tool to reproduce the experimental data

Completeness criteria

Criteria
C^c_1: Coverage of the target application domain
C^c_2: Spatial distribution of the experimental tests in the domain resulting from the intersection between the experimental and the target application domains

Best Estimate Plus Uncertainty International Conference (BEPU 2024)
Real Collegio, Lucca, Tuscany, Italy, May 19 – 24, 2024
BEPU2024-353

ADEQUACY ANALYSIS OF CRITICAL FLOW EXPERIMENTS IN THE FRAMEWORK OF THE OECD-NEA ATRIUM PROJECT: CEA'S CONTRIBUTION

Alberto Ghione, Lucia Sargentini, Guillaume Damblin, Philippe Fillion

Analytical Hierarchy Process (AHP)

- Multi-criteria decision analysis tool
- Goal: evaluate representativeness (rank exp. databases w.r.t. target application)
- Construction of matrixes via pairwise comparison (scale 1 to 9 by expert judgement) for:
  - Weight of each (sub-)criterion. Goal: identify the most important (sub-)criteria;
  - Exp. databases. Goal: obtain a weight for each database w.r.t. a (sub-)criterion.
- Based on these matrixes, we obtain vectors of:
  - Importance weights for each criterion
  - Representativeness scores for each exp. database associated to each criterion
- Via a weighted average of the representativeness scores per criterion → an unique representativeness score for each experimental database

	Cr_1	Cr_2	Cr_3
Cr_1	1	$1/S_{1,2}$	$1/S_{1,3}$
Cr_2	$S_{1,2}$	1	$1/S_{2,3}$
Cr_3	$S_{1,3}$	$S_{2,3}$	1

Representativeness: Quantification of the criteria weights

- Higher importance: high quality exp. data and reproducibility via a system code
- Less importance: fidelity w.r.t. target domain
- AHP → tendency to exaggerate differences

	Cr_1	Cr_2	Cr_3	weight
Cr_1	1	1/2	1/2	0.2
Cr_2	2	1	1	0.4
Cr_3	2	1	1	0.4

- Same weights to all sub-criteria

Representativeness: Comparison between exp. databases

- Pairwise comparison for each sub-criterion

Example: $C^r_{1\text{-}1}$ (Geometric fidelity)

	EXP1	EXP2	EXP3	EXP4	EXP5	EXP6	EXP7	weight
EXP1	1	8	2	1/3	2	2	9	0.2
EXP2	1/8	1	1/4	1/9	1/4	1/4	1	0.03
EXP3	1/2	4	1	1/6	1	1	3	0.09
EXP4	3	9	6	1	6	6	9	0.45
EXP5	1/2	4	1	1/6	1	1	4	0.1
EXP6	1/2	4	1	1/6	1	1	4	0.1
EXP7	1/9	1	1/9	1/9	1/9	1/9	1	0.02

- Weighted averages to obtain final score:

	C^r_1 Fidelity w.r.t. LSTF	C^r_2 Control of exp. data	C^r_3 Modelling of phenomena	Final score
EXP1	0.18	0.08	0.16	0.14
EXP2	0.04	0.08	0.03	0.05
EXP3	0.07	0.08	0.09	0.08
EXP4	0.50	0.28	0.37	0.36
EXP5	0.07	0.16	0.12	0.13
EXP6	0.07	0.16	0.12	0.13
EXP7	0.06	0.16	0.10	0.11
Weights	0.20	0.40	0.40	

Experimental data after the adequacy

	COSI	TOPFLOW	UPTF
Number of tests	315	24	24
Incorrect measurements	53	0	0
Non stabilized tests	14	0	0
No injection	71	0	0
Incomprehensible measurements	12	0	0
Repeated tests	8	0	0
Injection under the level of stratified liquid	6	2	0
Stratified injection	49	3	17
Data for the calibration	102	8	-
Data for the validation	-	11	7

From 363 test to 110 for the calibration and 18 for the validation

2. Model format selection: how physics is our best friend

Definition of the statistical problem

$$z_{exp}(x,\theta) = z_{pred}(x,M) + \varepsilon = \boxed{z_{calc}(x,\theta)} \cdot \Lambda(x) + \varepsilon$$

- z_{exp} ➔ experimental Quantity of Interest (QoI)
- x ➔ State variables (e.g. non-dimensional numbers, experimental conditions)
- θ ➔ Parameter
- z_{pred} ➔ predicted/simulated QoI
- M ➔ physical models depending on x, θ
- ε ➔ Experimental error: $\mathcal{N}(0, \sigma^2_{exp})$
- z_{calc} ➔ mathematical QoI, i.e. physical model
- Λ ➔ Model uncertainty ➔ **non reducible** with infinite experimental points

Definition of a physical model: an example

$$z_{calc}(x, \theta) = \theta_0 \cdot x_1^{\theta_1} \cdot x_2^{\theta_2}$$

mathematical QoI
or
Figure of Merit (FoM)

Parameters

« Uncertains »

State variables (e.g. non-dimensional numbers) **depend on physics**!!!!

This uncertainty is **reducible** with infinite experimental points

Choice of the format for the physical model

$$\eta_{calc}(\theta) = \theta_0 \cdot Nu_{pot,vap}^{\theta_1} \cdot {Re_{ECC}}^{\theta_2} \cdot Pr^{\theta_3}$$

Log-linearization !!!!!

$$\ln\left(\eta_{calc}(\theta)\right) = \ln(\theta_0) + \theta_1 \cdot \ln\left(Nu_{pot,vap}\right) - \theta_2 \cdot ln(Re_{ECC}) - \theta_3 \cdot ln(Pr)$$

Problem: find the $\boldsymbol{\theta}$ which fits at best the $\boldsymbol{z_{exp}}$

3. Model calibration: how statistics is our best friend

Simplified assumptions

1. The experimental error neglected ➔ Λ "contains" the experimental error

In nuclear domain, assumed to be "conservative"

$$z_{exp}(x,\theta) = z_{pred}(x,\theta) = z_{calc}(x,\theta) \cdot \Lambda(x)$$

2. The model uncertainty Λ is independent from x ➔ the uncertainty does not depend on experimental condition

$$z_{exp}(x,\theta) = z_{pred}(x,\theta) = z_{calc}(x,\theta) \cdot \Lambda$$

3. Λ is $\mathcal{LN}(\mathbf{0}, \boldsymbol{\sigma}_{\boldsymbol{\lambda}}^{\mathbf{2}})$ ➔ log-normal (log-gaussian) distribution with mean 0 and variance $\boldsymbol{\sigma}_{\boldsymbol{\lambda}}^{\mathbf{2}}$

Definition of the technical calibration

The uncertainty becomes addictive

Linearization

$$z_{exp}(x,\theta) = \Lambda \cdot z_{calc}(x,\theta) \Leftrightarrow \ln\left(z_{exp}\right) = \ln\left(z_{calc}(x,\theta)\right) + \ln(\Lambda) \Leftrightarrow \ln\left(z_{exp}\right) = h^T \cdot \boldsymbol{\theta} + \ln(\Lambda)$$

With Bayes' theory ➔ $\boldsymbol{\theta}^{MAP}$ and $\boldsymbol{\sigma}^2$

$$ln(\Lambda) \sim \mathcal{N}(0,\sigma^2)$$

MAP: Maximum a Posteriori ➔ the best value to fit!

Process of the technical calibration

The uncertainty becomes addictive

Linearization

$$z_{exp}(x,\theta) = \Lambda \cdot z_{calc}(x,\theta) \Leftrightarrow \ln(z_{exp}) = \ln(z_{calc}(x,\theta)) + \ln(\Lambda) \Leftrightarrow \ln(z_{exp}) = h^T \cdot \boldsymbol{\theta} + \ln(\Lambda)$$

$$ln(\Lambda) \sim \mathcal{N}(0,\sigma^2)$$

Estimation		
Bayes' theory	Parameters' distribution	Maximum a posteriori MAP

Selection and validation	
Validation of assumptions	Statistical indicators

Prediction	
Prediction of MAP	Uncertainty quantification

Bayes' theorem

A and B: events ➔ A is the proposition
B is the evidence

Likelihood function: probability of the evidence B supports the proposition A

Posterior probability distribution: probability of the evidence A after taking into account B

$$\pi(A|B) = \frac{\pi(B|A)\,\pi(A)}{\pi(B)}$$

Prior probability distribution: beliefs about A or B before evidence is taken into account

Bayes' theorem

A ➔ θ, σ^2 ➔ random variable
B ➔ $z_{exp}(x)$

Likelihood function

What we can manage

Defined depending by assumptions (e.g. Jeffrey's prior)
Prior probability distribution

Posterior probability distribution

What we want to find!

$$\pi\left(\theta, \sigma^2 \middle| \ln(z_{exp}(x))\right) = \frac{\mathcal{L}\left(\ln(z_{exp}(x)) \middle| \theta, \sigma^2\right) \pi(\theta, \sigma^2)}{\pi(\ln(z_{exp}(x)))}$$

With some statistical considerations, we can find σ^2 after finding the best θ, i.e. θ^{MAP}

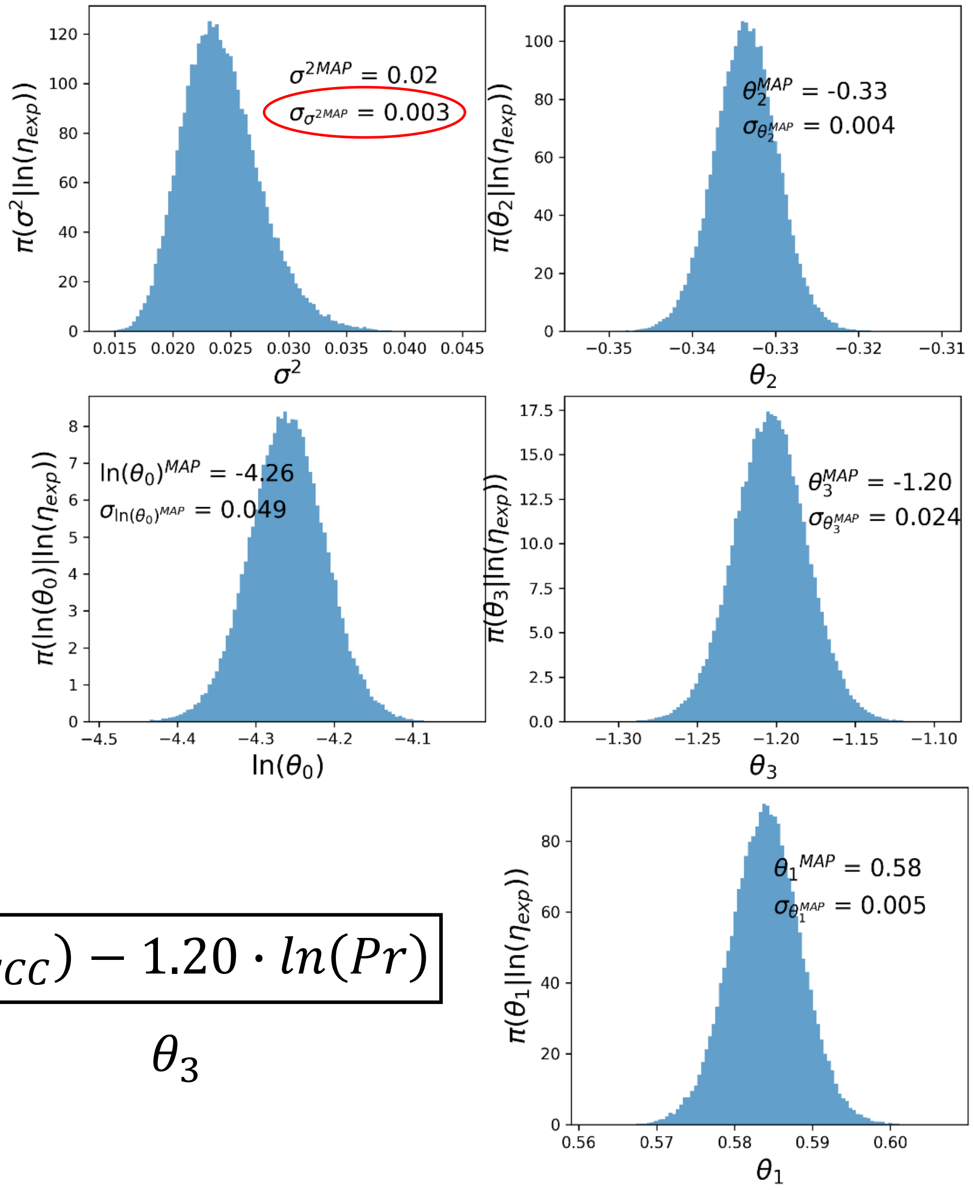
Parameters' estimation

$$\eta_{calc}(\theta) = \theta_0 \cdot Nu_{pot,vap}^{\theta_1} \cdot Re_{ECC}{}^{\theta_2} \cdot Pr^{\theta_3}$$

1. Log-linearization of the model
2. Jeffrey's prior distribution
3. Application of Bayes' theorem
4. Definition of Maximum A Posteriori (MAP) value

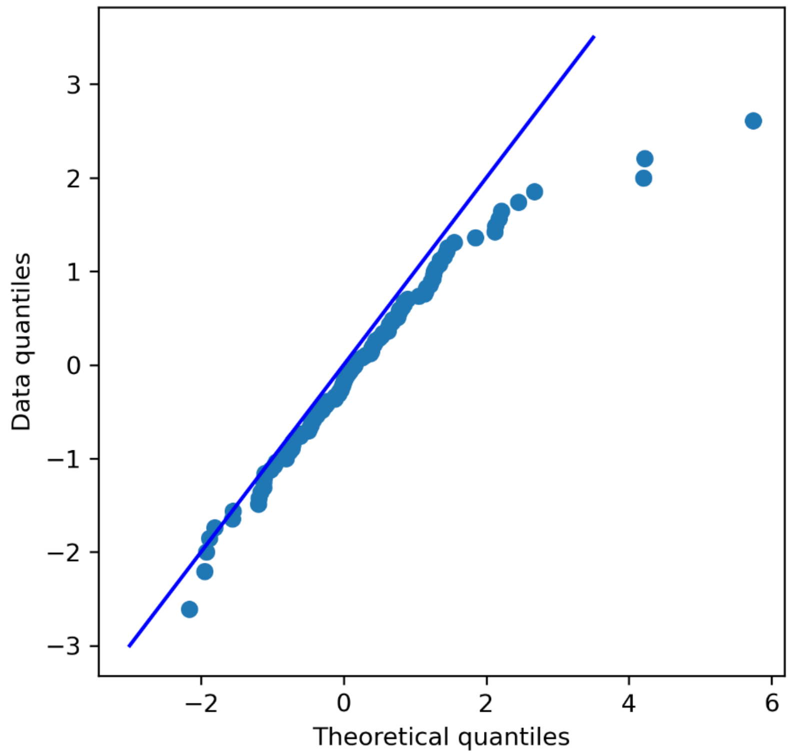
$$\ln\left(\eta_{calc}(\theta^{MAP})\right) = -4.26 + 0.58 \cdot \ln\left(Nu_{pot,vap}\right) - 0.33 \cdot ln(Re_{ECC}) - 1.20 \cdot ln(Pr)$$

$\ln \theta_0$ θ_1 θ_2 θ_3



Statistical validation

$$\eta_{calc}(\theta^{MAP}) = 0.014 \cdot Nu_{pot,vap}^{0.58} \cdot Re_{ECC}^{-0.33} \cdot Pr^{-1.2}$$



R-squared: measure of goodness of fit

Adjusted R-squared: measure of goodness of fit depending on the number of variables

Relative residual: relative error in percentage

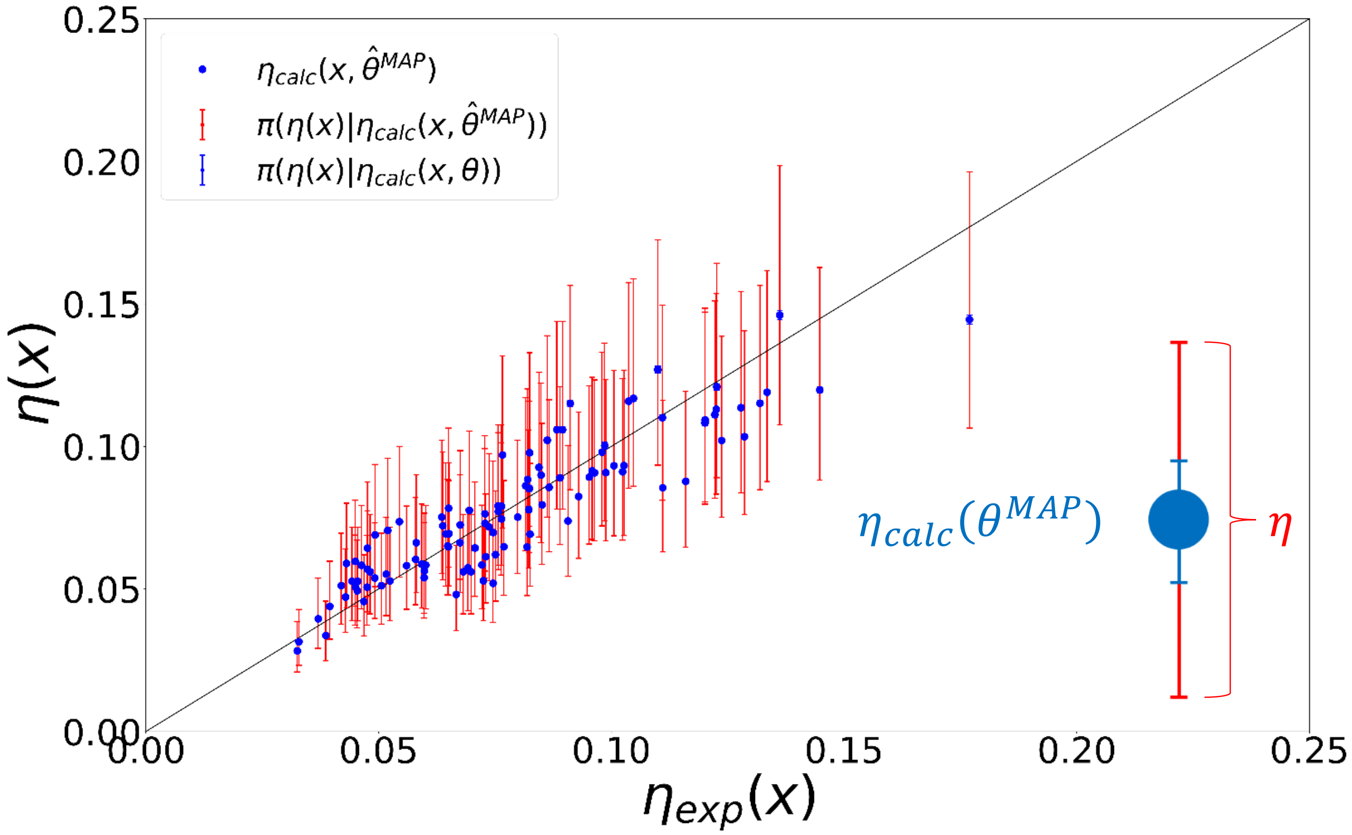
Absolute residual: absolute error

Bayesian Information Criterion (BIC): statistical indicator based on the MAP and penalised by the number of the model unknown parameters p.

$$BIC(\theta^{MAP}) = -2\ \ln\left(\mathcal{L}\left(\ln Nu_{exp}\,|\theta^{MAP}\right)\right) + p\ \ln n$$

p: number of parameters(p=5)
n: number of tests (n=110 essais)

Uncertainty quantification of the model prediction



The uncertainty of θ is negligeable

The uncertainty of the physical model is $\sigma^{2^{MAP}}$

0.023

$$\eta = \lambda \cdot \eta_{calc}(\theta^{MAP}) \text{ où } \lambda \sim \mathcal{LN}(0, \sigma^{2^{MAP}})$$

$$IF_{95\%}(\lambda) = \left[e^{-1.96 \cdot \sqrt{\sigma^{2^{MAP}}}}, e^{1.96 \cdot \sqrt{\sigma^{2^{MAP}}}}\right] = [0.74, 1.35]$$

Uncertainty on assessed model

“ R. Cocci, A. Ghione, L. Sargentini, G. Damblin and D. Lucor, Model Assessment for Direct Contact Condensation Induced by a Sub-cooled Water Jet in a Circular Pipe, International Journal of Heat and Mass Transfer 195, 123162, 2022, https://www.sciencedirect.com/science/article/pii/S0017931022006329

R. Cocci et al., Extension of the CIRCE methodology to improve the Inverse Uncertainty Quantification of several combined thermal-hydraulic models, Nuclear Engineering and Design, Volume 398, 2022, 111974, ISSN 0029-5493, https://doi.org/10.1016/j.nucengdes.2022.111974. (https://www.sciencedirect.com/science/article/pii/S0029549322003259)

Definition of the statistical problem

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Necessary assumptions

- The code is verified and validated
- Separate Effect Tests shall be sensitive to models ! Sensitivity analysis on the SETs allows to define which correlations are influent *(Prior Sensitivity Analysis)*

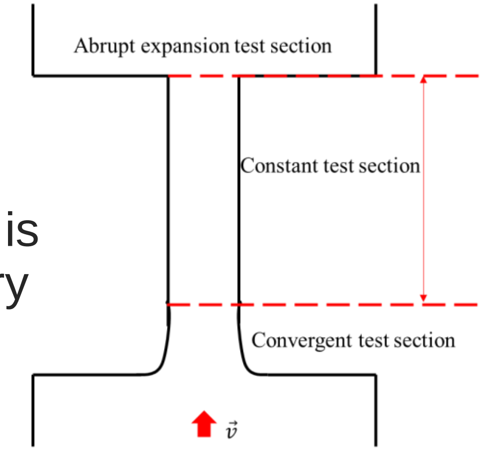
Description of SETs

L. Sargentini and G. Damblin. Sensitivity analysis on the critical mass flowrate based on Sobol’ indices through replicated LHS. In 18th International Topical Meeting on Nuclear Reactor Thermal Hydraulics (NURETH-18), August 2019.

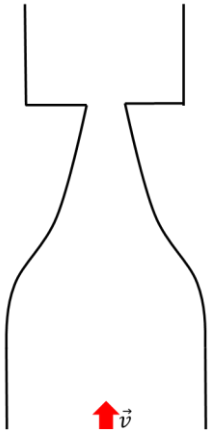
SETs to evaluate the chocked mass flow on a vertical pipe

94 experimental tests

Two areas of test section: Geometry A1 is smaller than Geometry A2



a) Geometry A: BETSHY-nozzle



a) Geometry B: Super MobyDick

	BETSHY-Nozzle (Geometry A)	SMD (Geometry B)
Pressure [Mpa]	3-10	2-8
Temperature [°C]	204-310	192-294
Quality	Up to 0.2	Up to 0.02

Which models for the prior sensitivity analysis?

Simulations performed with the TH-system code CATHARE

After a physical analysis on the critical mass flow rate, 5 models are defined:

- Wall-to-liquid friction factor : SP1
- Flashing : SP2
- Delay flashing : SP3
- Interfacial friction factor : SP4
- Steam-to-liquid friction model : SP5

Verify the influence of these models on the database

Which methodology to quantify the relevance of a model?

Sobol’ first order indices through replicated Latin Hypercube Sampling (rLHS)

Quantifying the relevance with a variance-based index computed by the pick and freeze sampling

Obtaining the whole set of first order indices with only **2N number of simulations** instead of N(p+1) BUT poor estimation of small indexes

Three values to check:

Value of each Sobol’ first order index of the sensitivity parameter for every experimental tests

Influence of the variation of the sensitivity parameters on the QoI for each experimental test

Sum of the Sobol’ first order index for each experimental test

Application on the SETs

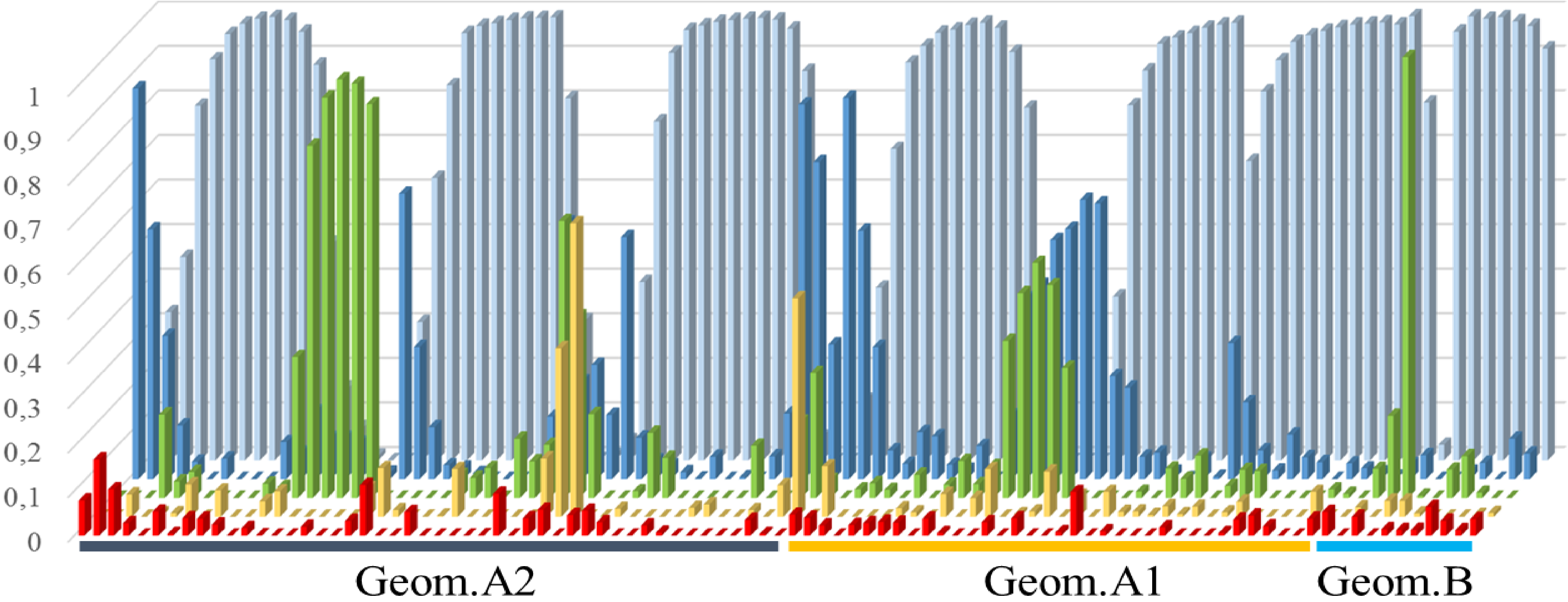
Uncertainties propagation with URANIE platform

Every sensitivity parameters ➔uniform distribution [0,5 ; 2]
N = 500 (x2) performed for every experimental tests

QoI is the critical mass flow rate

Sensitivity on the number calculations was realized

Sobol' first indices for every experimental test

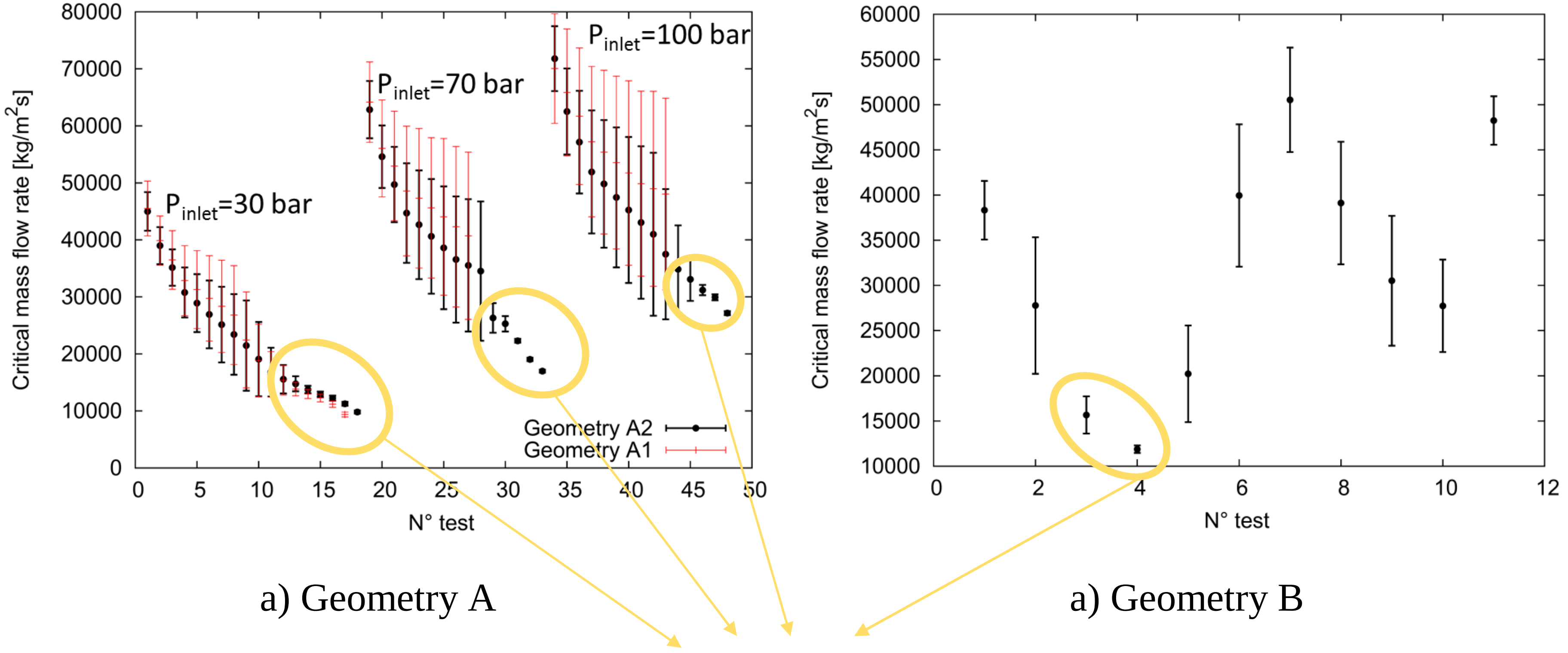


- Wall-to-liquid friction factor: **SP1**
- Flashing: SP2
- Delay flashing: **SP3**
- Interfacial friction factor: **SP4**
- Steam-to-liquid friction model: SP5

Many tests are sensitive to the flashing model
Some tests are sensitive to the interfacial friction or the wall-to liquid friction

Influence of all sensitivity parameters on the QoI

Bars in the plots represent the variation of the QoI respect to the variation of all SP



a) Geometry A

a) Geometry B

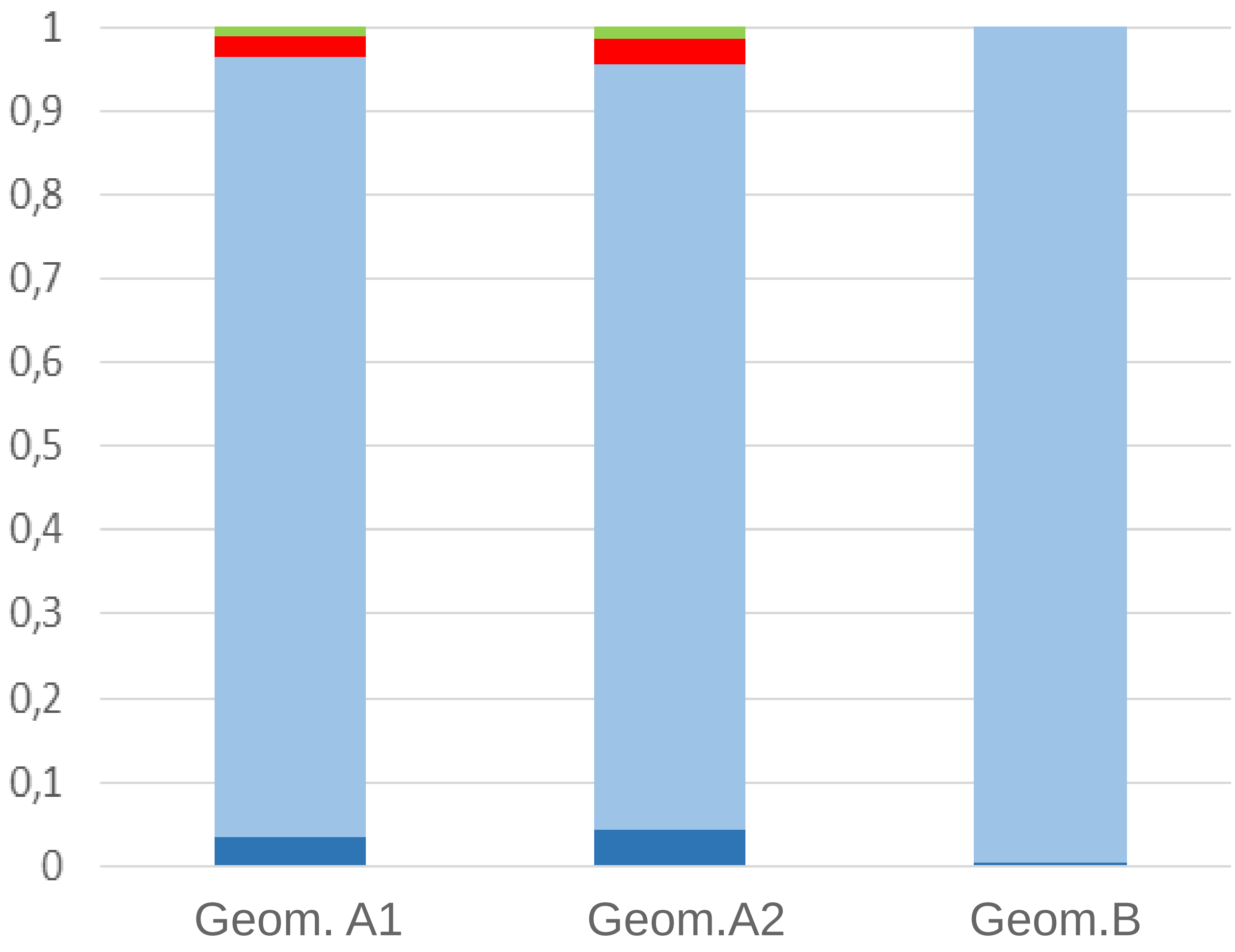
No influence of the variation of the SP on the QoI

Tests with interfacial friction sensitivity SP5

Sum of the first order sobol' indices

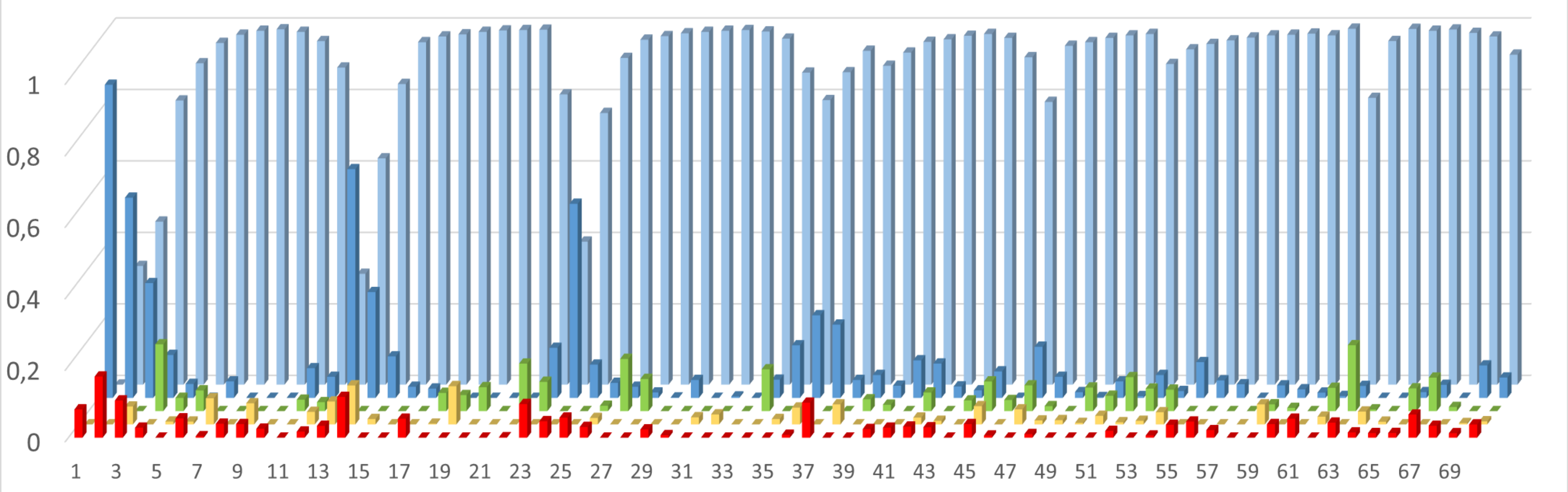
- Wall-to-liquid friction factor: **SP1**
- Flashing: SP2
- Delay flashing: **SP3**
- Interfacial friction factor: **SP4**
- Steam-to-liquid friction model: SP5

No interactions between models



Sobol' indices of the reduced database

Wall-to-liquid friction: **SP1** Flashing: **SP2** Delay flashing: **SP3**
Interfacial friction: **SP4** Steam-to-liquid friction: **SP5**



70 tests

With this database (without tests in which SP1 is relevant), the inverse uncertainties quantification **only** for the flashing model of CATHARE2 can be assessed

The need of a prior sensitivity analysis:

The ranking of the database allows to perform the inverse uncertainties quantification on a database which is sensitive to the model !!!

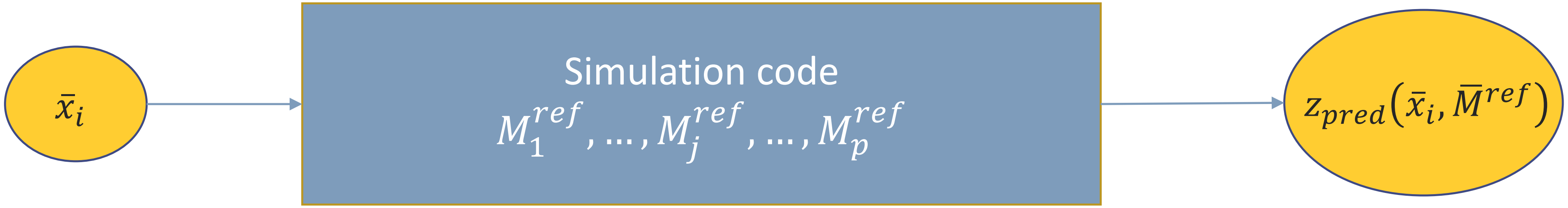
Necessary assumptions

- The code is verified and validated
- The physical model for which we want to quantify the uncertainty is sensitive enough w.r.t. the output
- The experimental data are adequate in the sense of the ATRIUM project definition

The uncertainty of the prediction

Codes are full of **physical models/closure laws ➔ uncertain** because of lack of knowledge

Every code is based on *j*-th physical models, defined as $\boldsymbol{M_j^{ref}}$, depending on i-th experimental conditions *x*



$$M_j^{\Lambda}(\bar{x}) = \Lambda_j \cdot M_j^{ref}(\bar{x})$$

How define it?

Inverse Uncertainty Quantification

Estimation of the uncertainty of physical models from the error between simulation and experiments

$$\varepsilon = z_{exp}(x, \theta) - z_{pred}(x, M) \cdot \Lambda_j$$

The IUQ methodology

Uncertainty Modelling of Input Factors + Technical estimation

- reducible with infinite data ➔ calibration
- non reducible with infinite data ➔ quantification

DoE, Bayesian,
Frequentist, Data Assimilation

X. Wu, Z. Xie, F. Alsafadi, and T. Kozlowski. A comprehensive survey of inverse uncertainty quantification of physical model parameters in nuclear system thermal–hydraulics codes. Nuclear Engineering and Design, 384:111460, 2021.

$$M_j^{\Lambda}(\bar{x}) = \Lambda_j \cdot M_j^{ref}(\bar{x})$$

Λ= inter-variability (pdf : mean, variance) ➔ CEA used CIRCE methodology

CIRCE Methodology: Brief description

$$M_j^{\Lambda}(\bar{x}) = \Lambda_j \cdot M_j^{ref}(\bar{x})$$

$$\Lambda_j \sim N(m, \sigma^2) \qquad \Lambda_j \sim \mathcal{L}N(m, \sigma^2)$$

- Estimation of the (log-)normal distribution of the uncertain model parameters
- Discrepancies between experimental and calculated values of the QoI are modelled as:

$$\varepsilon = z_{exp}(x, \theta) - z_{pred}(x, M) \cdot \Lambda_j$$

$$\varepsilon = \mathcal{N}(0, \sigma_{exp}^2)$$

Conservative hypothesis

- Aleatory modelling of input factors + Frequentist IUQ estimation (Maximum Likelihood Estimation MLE)

- Hyp: (log-)linearity of code output to input variation + normality of standardized residuals

The CIRCE methodology

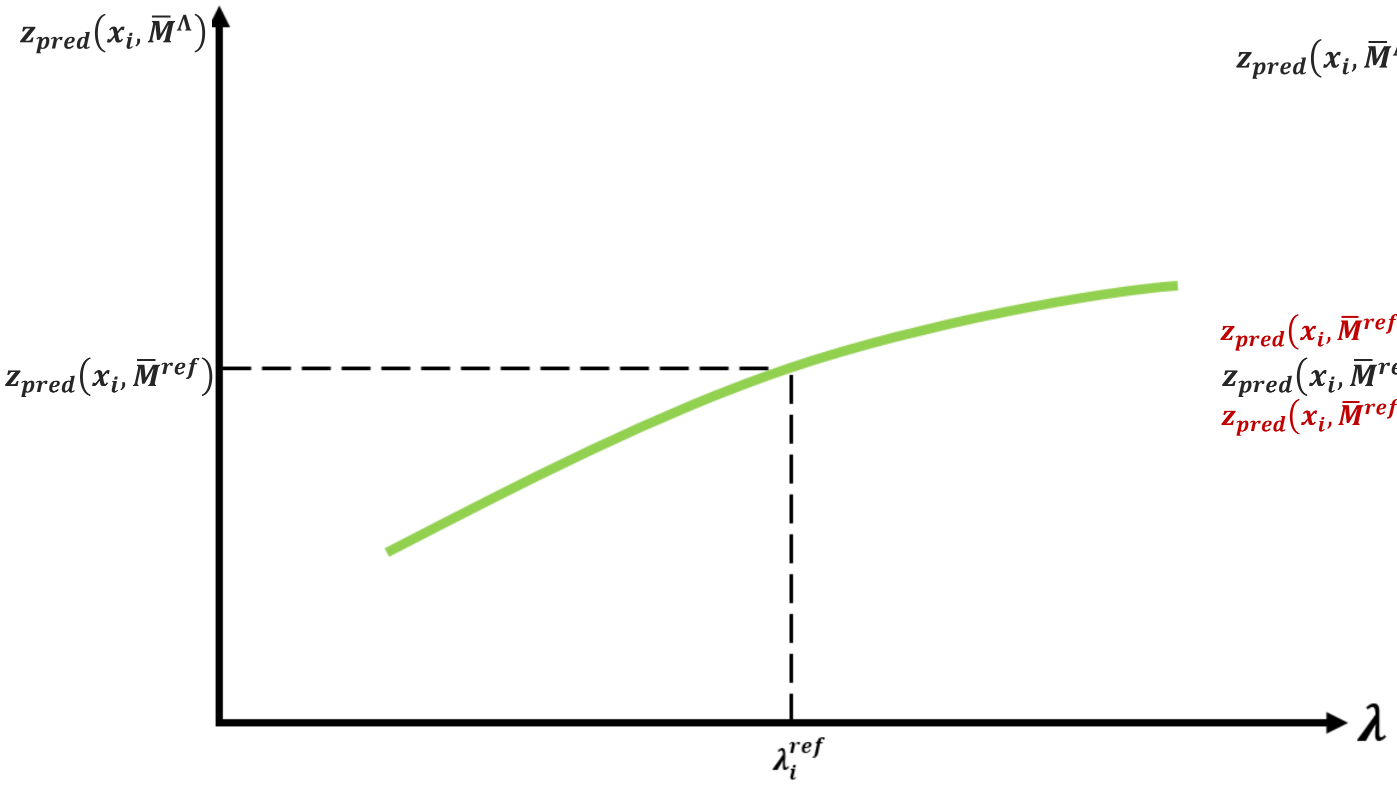
$$z_{exp}(x, \theta) = z_{pred}(x, M) \cdot \Lambda_j$$

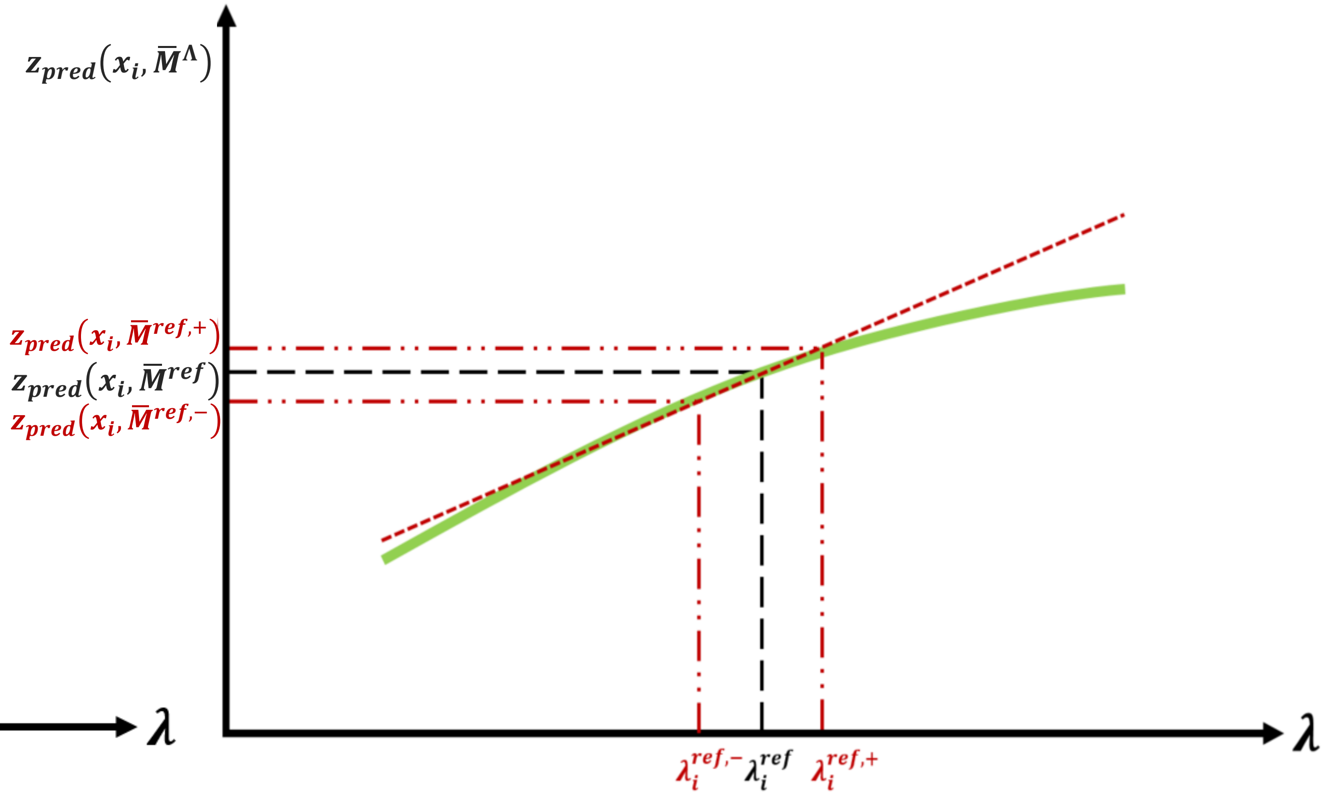
The realization of every $\boldsymbol{\lambda_{j,i} \sim \Lambda_j}$ is not explicit

⬇

We can find $\boldsymbol{\lambda_{j,i} \sim \Lambda_j}$ with the linearization of the code response $\boldsymbol{z_{pred}}(\boldsymbol{x_i}, \boldsymbol{\bar{M}^{\Lambda}})$ w.r.t. $\boldsymbol{\Lambda_j}$

First step: linearization of the code





$$z_{exp}(x_i) = z_{pred}(x_i, \bar{M}^{\Lambda}) + \varepsilon_i$$

"Perturbation" of the code response w.r.t. λ_i^{ref} = 1

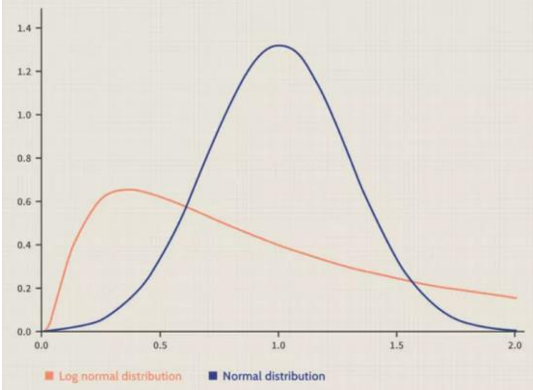
$$z_{exp}(x_i) \approx z_{pred}(x_i, \bar{M}^{ref}) + \bar{h}_i \cdot \bar{b}_i^T + \varepsilon_i$$

$$\bar{h}_i = \frac{z_{pred}(x_i, \bar{M}^{ref,+}) - z_{pred}(x_i, \bar{M}^{ref,-})}{\lambda_i^{ref,+} - \lambda_i^{ref,-}}$$

$$\bar{b}_i^T = \left(\lambda_i - \lambda_i^{ref}\right)^T$$

Derivative ➔ sensitive!!!!!!

Second step: the Expectation/Conditional Maximisation Either (ECME) algorithm



$$z_{exp}(x,\theta) = z_{pred}\left(x_i, M^{ref}\right) + \overline{h}_i \cdot \boldsymbol{\overline{b}_i^T}$$

Known quantity

Unknown quantity

The realization of the bias $\overline{b}_i$ are (log-)normal : $\boldsymbol{\overline{b}_i \sim \overline{b} = \mathcal{N}(\overline{m}_b, \Sigma_b)}$ $\boldsymbol{with\ \Sigma_b = diag\left(\sigma_{b_1}^2, \dots, \sigma_{b_j}^2, \dots, \sigma_{b_p}^2\right)}$

The ECME algorithm estimates the optimal parameters of the Gaussian vector $(\overline{m}_b^{MLE}, \Sigma_b^{MLE})$

After estimating $\overline{b}$, let's come back on $\boldsymbol{\lambda}$!

$$b_j = \mathcal{N}(m_{b_j}^{MLE}, \sigma_{b_j}^{2,MLE}) \rightarrow \lambda \rightarrow \Lambda_j = \mathcal{N}(m_{b_j}^{MLE} + 1, \sigma_{b_j}^{2,MLE})$$

$$b_j = \mathcal{N}(m_{b_j}^{MLE}, \sigma_{b_j}^{2,MLE}) \rightarrow log(\lambda) \rightarrow \Lambda_j = \mathcal{LN}(m_{b_j}^{MLE}, \sigma_{b_j}^{2,MLE})$$

Application of CIRCE

1. Download URANIE ➔ https://www.salome-platform.org/?page_id=2019

2. Create the *filename.dat* ➔

z_{exp} | z_{pred} | $\bar{h}_i$

```
1 #NAME: circe
2 #TITLE:       DATA AND CALCULATIONS
3 #DATE:08-Jan-2019
4 #COLUMN_NAMES:
5
6 191.9     187.4     91.902714
7 214.4     223.5     83.17552735
8 201.0     196.4     89.69662345
9 227.5     233.2     77.5811087
10 227.2    232.6     76.7114808
11 218.7    214.4     83.9457811
12 223.3    213.9     82.8006746
13 220.2    202.5     84.9564742
14 218.5    227.1     81.16503875
15 215.7    218.0     84.20573885
16 212.1    199.7     87.14251035
17 210.9    206.4     85.61810535
18 135.1    135.4     65.04692645
```

Application of CIRCE

1. Download URANIE ➔ ht
2. Create the *filename.dat*
3. Create the *filename.C* ➔

```
{
  TDataServer * tds = new TDataServer();
  tds->fileDataRead("   filename.dat   ");

  TCirce * tc = new TCirce(tds,   "z_exp", "z_pred", "h_i"   );

  tc->estimate();

// Je termine CIRCE et je l'Ã©cris
  cout<< "End of CIRCE estimation"<<endl;
  tds->exportData("   filename.dat   ");
// Je recupere le vecteur bias et la matrice de variance et je l'imprime
 TVectorD Biais = tc -> getBVector();
  TMatrixD varBiais  = tc-> getMatrixVarianceMu();
  //   cout<< "Variance Matrix"<<endl;
  TMatrixD Variance    = tc -> getCMatrix(); //>> matc.txt;
  TMatrixD varVariance = tc -> getMatrixVarianceSigma();
  Variance.Print();
  varVariance.Print();
//
  Double_t Variance_SCOQLES    = Variance(0,0);
  Double_t varVariance_SCOQLES = varVariance(0,0);
//  Double_t Variance_PQST       = Variance(1,1);
//  Double_t varVariance_PQST    = varVariance(1,1);
//
 cout << "%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%" << endl;
 cout << " Moyenne_SCOQLES = "  << TMath::Exp(Biais(0)) << endl;
 cout << " ecart-type_SCOQLES = " << TMath::Sqrt(Variance_SCOQLES) << endl;
//  cout << " Moyenne_PQST = "  << Biais(1) << endl;
//  cout << " ecart-type_PQST = " << TMath::Sqrt(Variance_PQST) << endl;
//  cout << "Complete Analysis"<<endl;
 cout << "--------------------------------------------------------------------------" << endl;
}
```

Application of CIRCE

1. Download URANIE ➔ https://www.salome-pl
2. Create the *filename.dat*
3. Create the *filename.C*
4. Write on a terminal in Linux:
   root *filename*.C
5. Results on $(m_{b_j}^{MLE}, \sigma_{b_j}^{2,MLE})$

```
 ** matrix C1

1x1 matrix is as follows

     |      0    |
------------------
   0 |     0.0431


 ** vector XM1

Vector (1)  is as follows

     |        1  |
------------------
   0 |0.0204155

 ** End Of Initial Matrix C [1/1]
 **********************************
 ** Residual :: Mean [1.974821486280146e-16] Std[1.004454365030374]
End of CIRCE estimation

1x1 matrix is as follows

     |      0    |
------------------
   0 |     0.0431


1x1 matrix is as follows

     |      0    |
------------------
   0 |  3.288e-05

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
 Moyenne_biais = 0.020415456493840 91
 Moyenne_Lambda = 1.020625277356155
 ecart-type_Lambda = 0.2076018656992598
 variance_Lambda = 0.0430985346418135
------------------------------------------------------------------------
```

$\sigma_{b_j}^{2,MLE}$ (beside the first 1x1 matrix)

$m_{b_j}^{MLE}$ (beside the vector)

$\sigma_{b_j}^{2,MLE}$ (beside the second 1x1 matrix)

$\sigma^2(\sigma_{b_j}^{2,MLE})$ (beside the third 1x1 matrix)

Application of CIRCE

1. Download URANIE ➔ https://www.salome-platform.org/?page_id=2019

2. Create the *filename.dat*

3. Create the *filename.C*

4. Write on a terminal in Linux:
   root filename.C

5. Results on $(m_{b_j}^{MLE}, \sigma_{b_j}^{2,MLE})$

6. Depending on λ ➔ λ ➔ $\Lambda_j = \mathcal{N}(m_{b_j}^{MLE} + 1, \sigma_{b_j}^{2,MLE})$

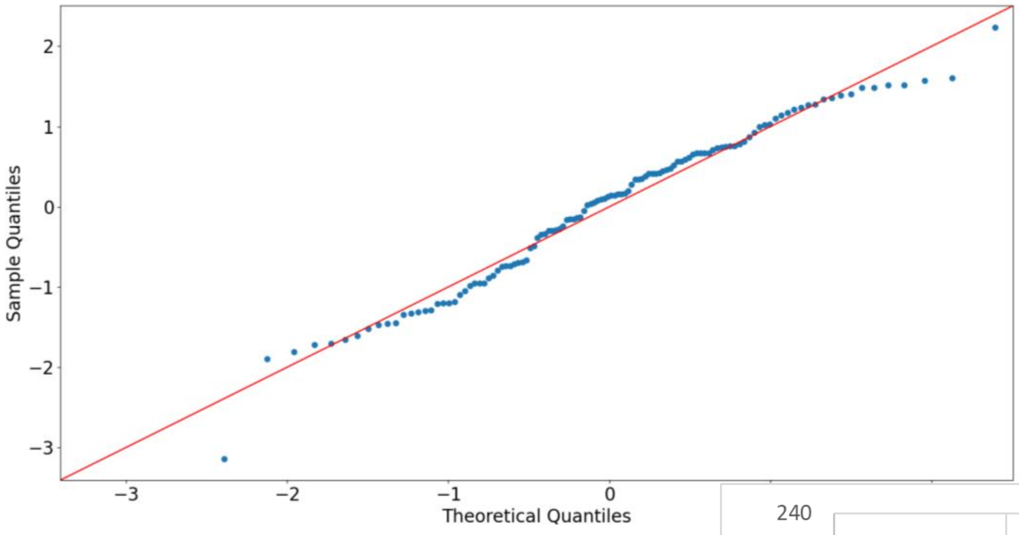
   $log(\lambda)$ ➔ $\Lambda_j = \mathcal{LN}(m_{b_j}^{MLE}, \sigma_{b_j}^{2,MLE})$

In the example: $\Lambda_j = \mathcal{LN}(1.03, 0.2076)$

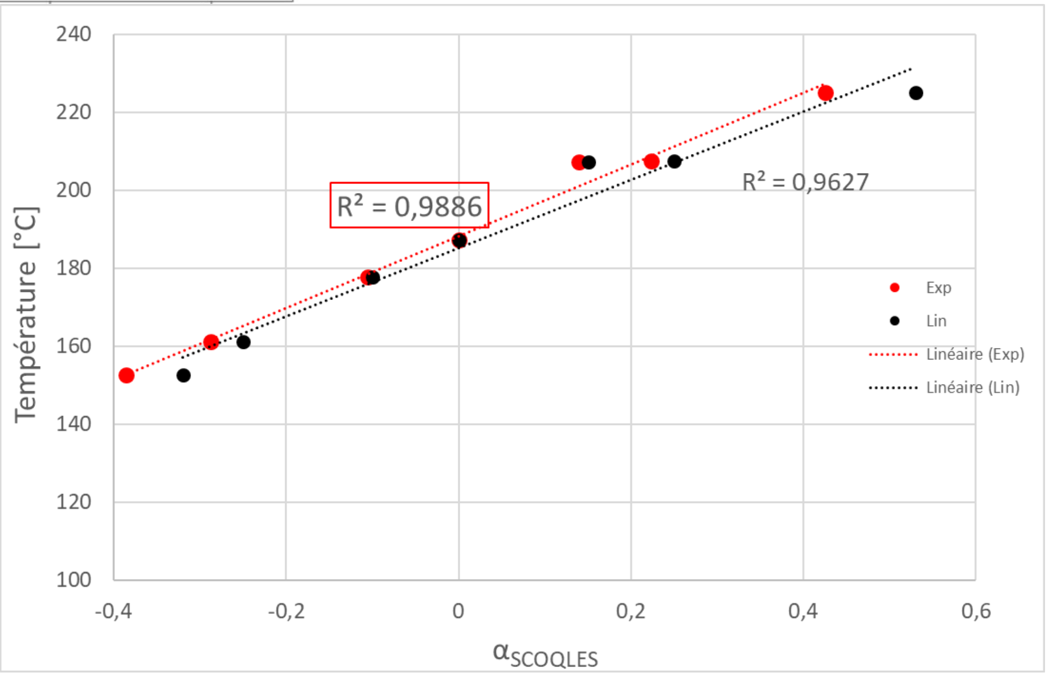
$$IF_{95\%} = [0.68, 1.53]$$

Two hypothesis to be verified

1. Normality of vector $\bar{b}$

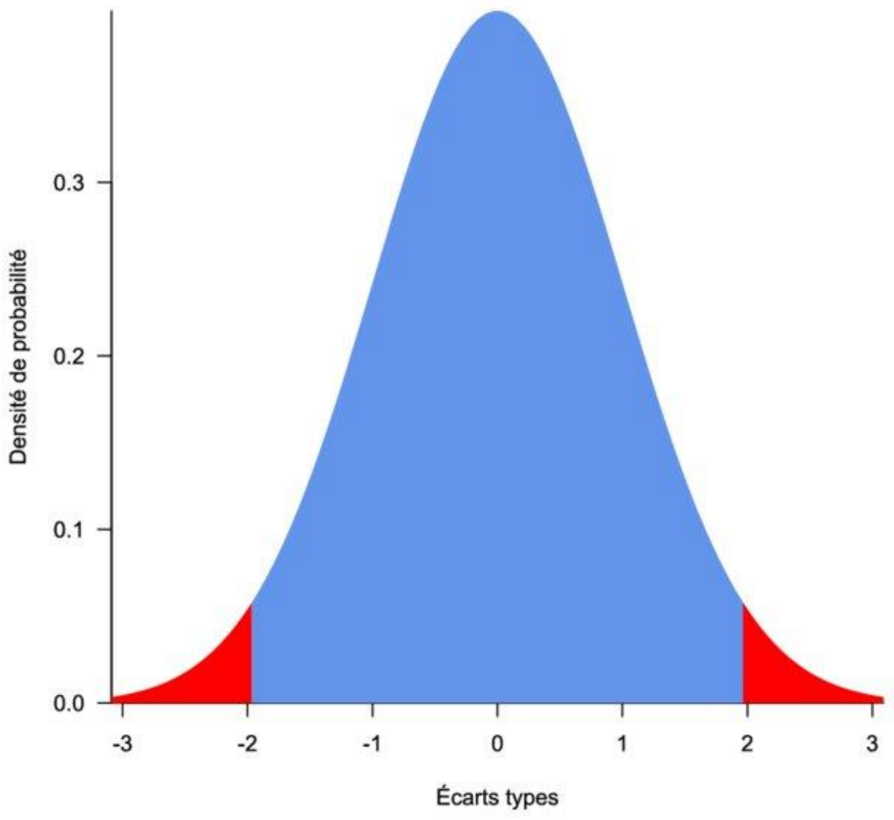


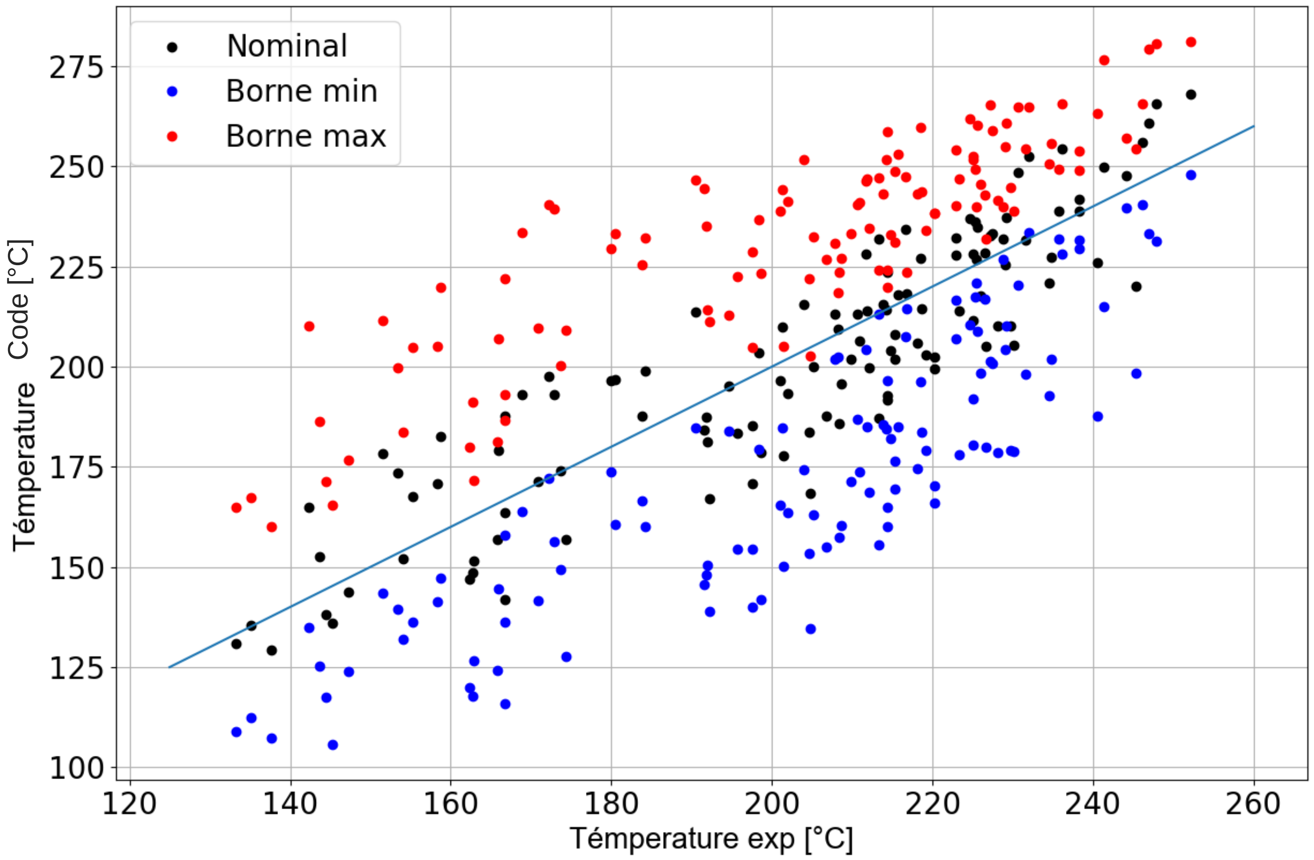
2. Linearization of the code response w.r.t. λ or $log(\lambda)$



Confirmation and validation of the uncertainty

1. Confirmation ➔ 95% if the experimental **data used to assess** the uncertainty are in the 95%/95% interval
2. Validation ➔ 95% if the experimental data **NOT used to assess** the uncertainty are in the 95%/95% interval





Conclusion

- Uncertainty are the cherry on the cake of the V&V
- Experimental data are fundamental
- Several methodologies exist for IUQ ➔ CIRCE is one of the most used (others CIRCE
- Uncertainty needs physics and physics needs uncertainty

Thank you!

Statistical methodology for uncertainty quantification/propagation for materials

Lucia SARGENTINI, PhD

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91191, Gif-sur-Yvette

1. Calibration under uncertainty

The importance of the experimental data

The importance of the physics

The importance of the statistical model

2. Uncertainty of assessed model

The importance of sensitivity analysis

The importance of the statistical model for the quantification of uncertainty

cea