Forward and Inverse Uncertainty Quantification of Thermal-Hydraulics Physical Model Parameters

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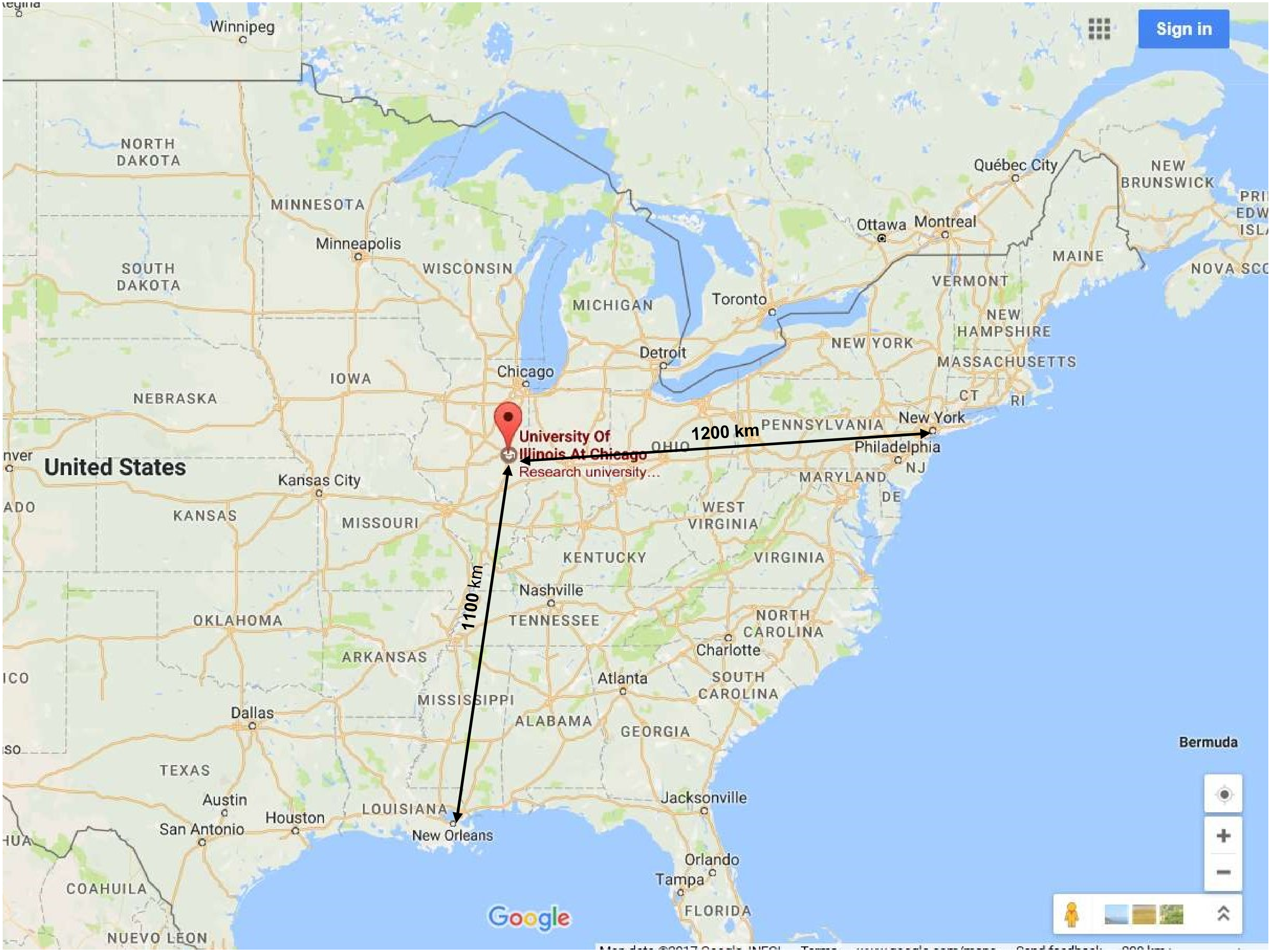
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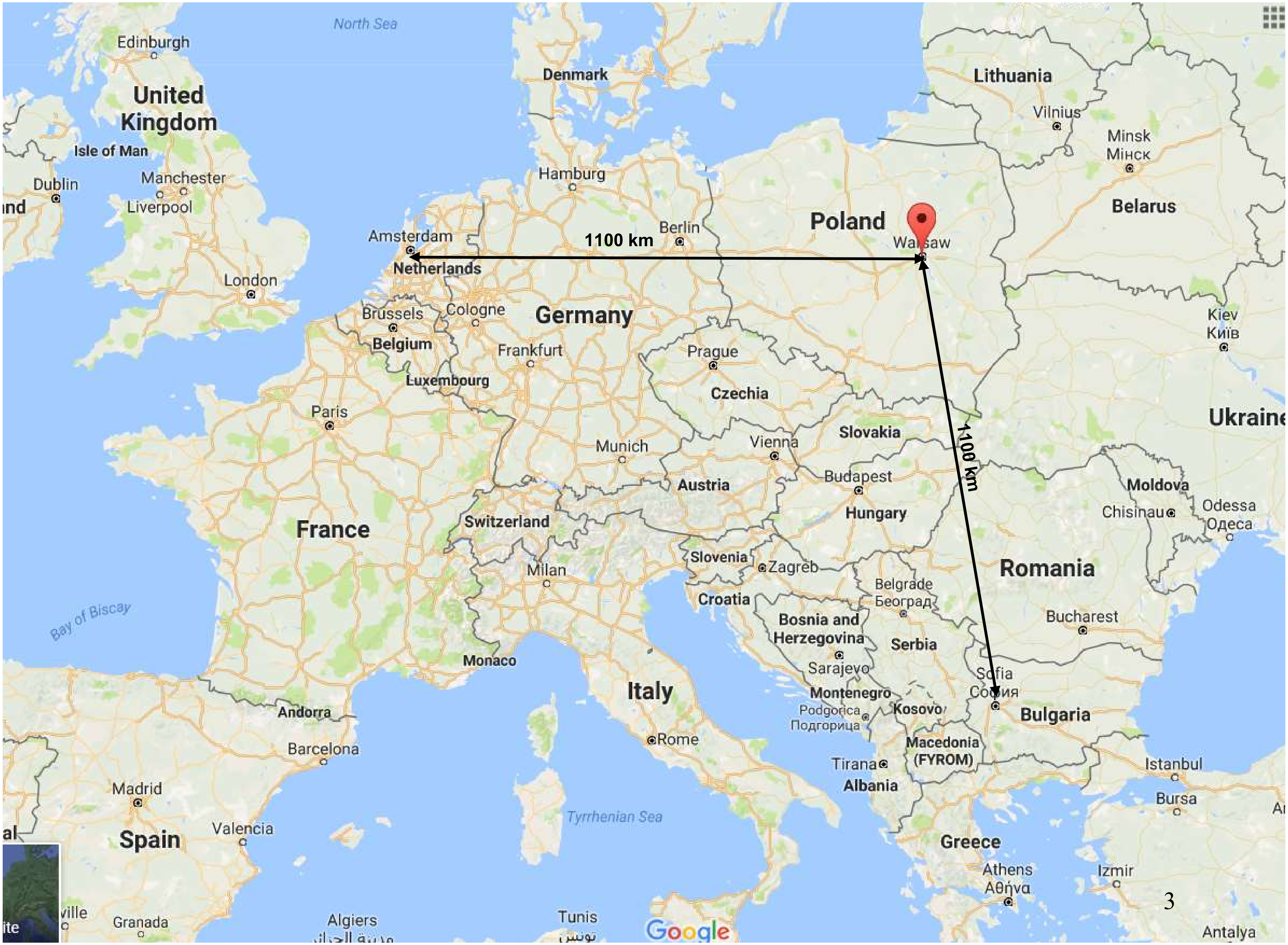
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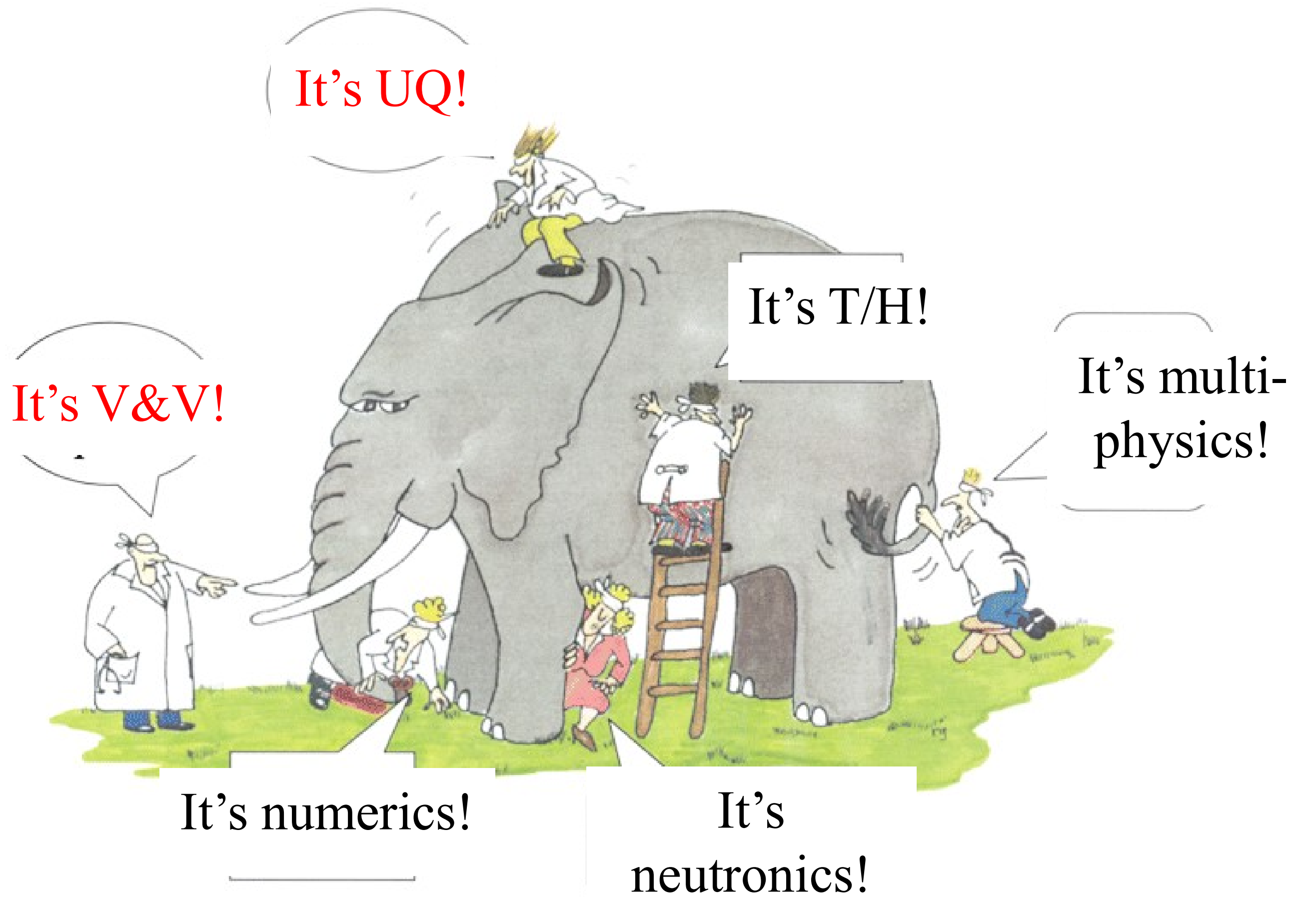
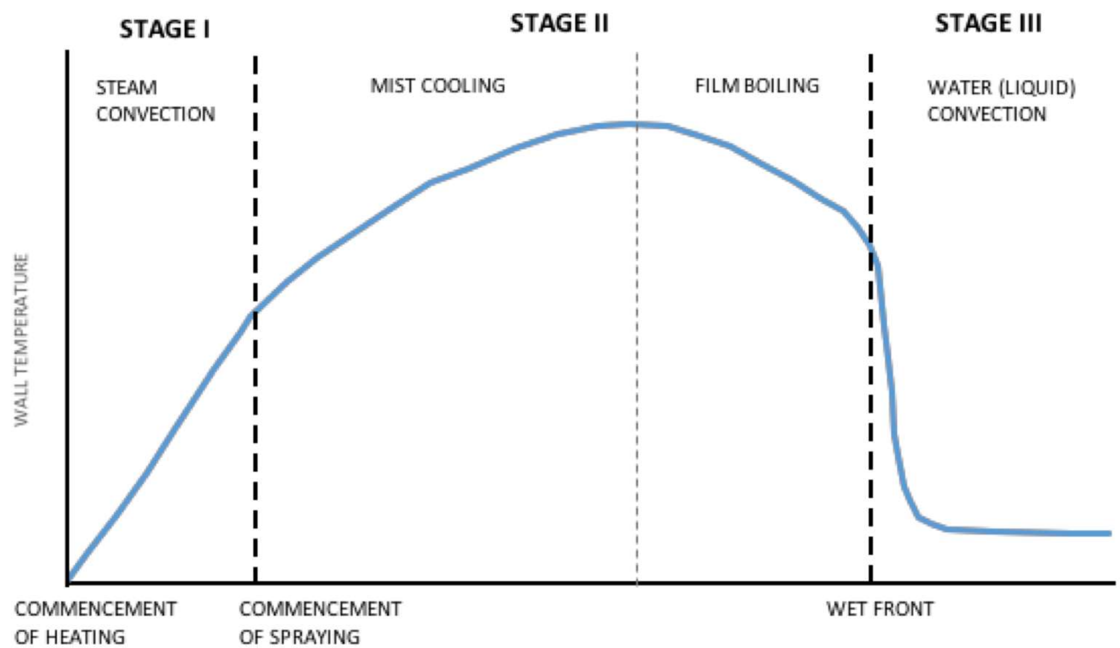
Typical scientific discussion…

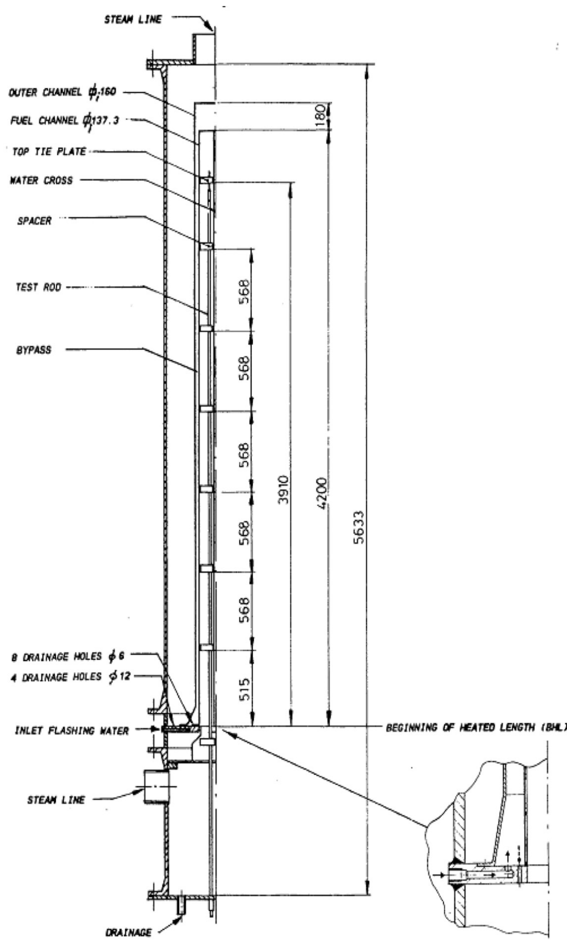


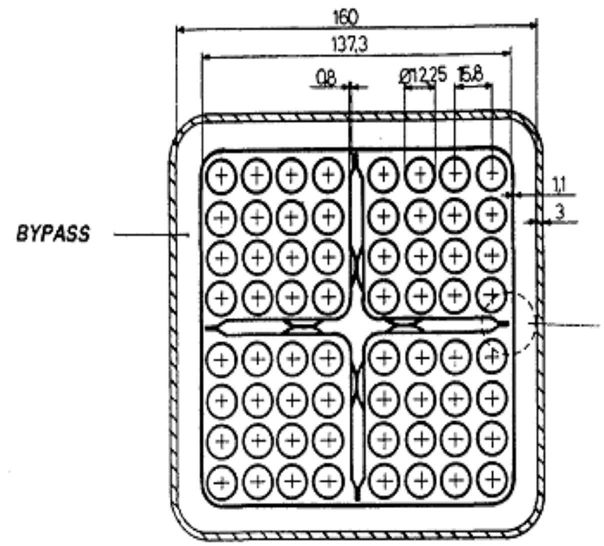
Post-LOCA BWR Spray Cooling

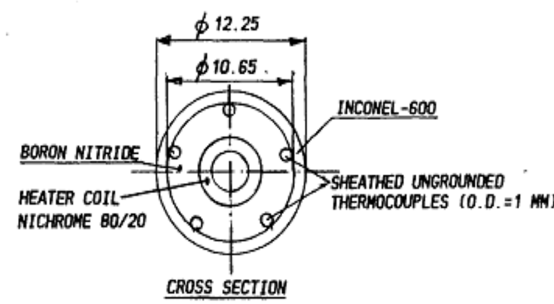
- ♦ Stage I – steam convection (end of blowdown)
- ♦ Stage II – DFFB and post-CHF flow cooling (refill-reflood)
- ♦ Stage III – water film quench, annular flow (reflood)



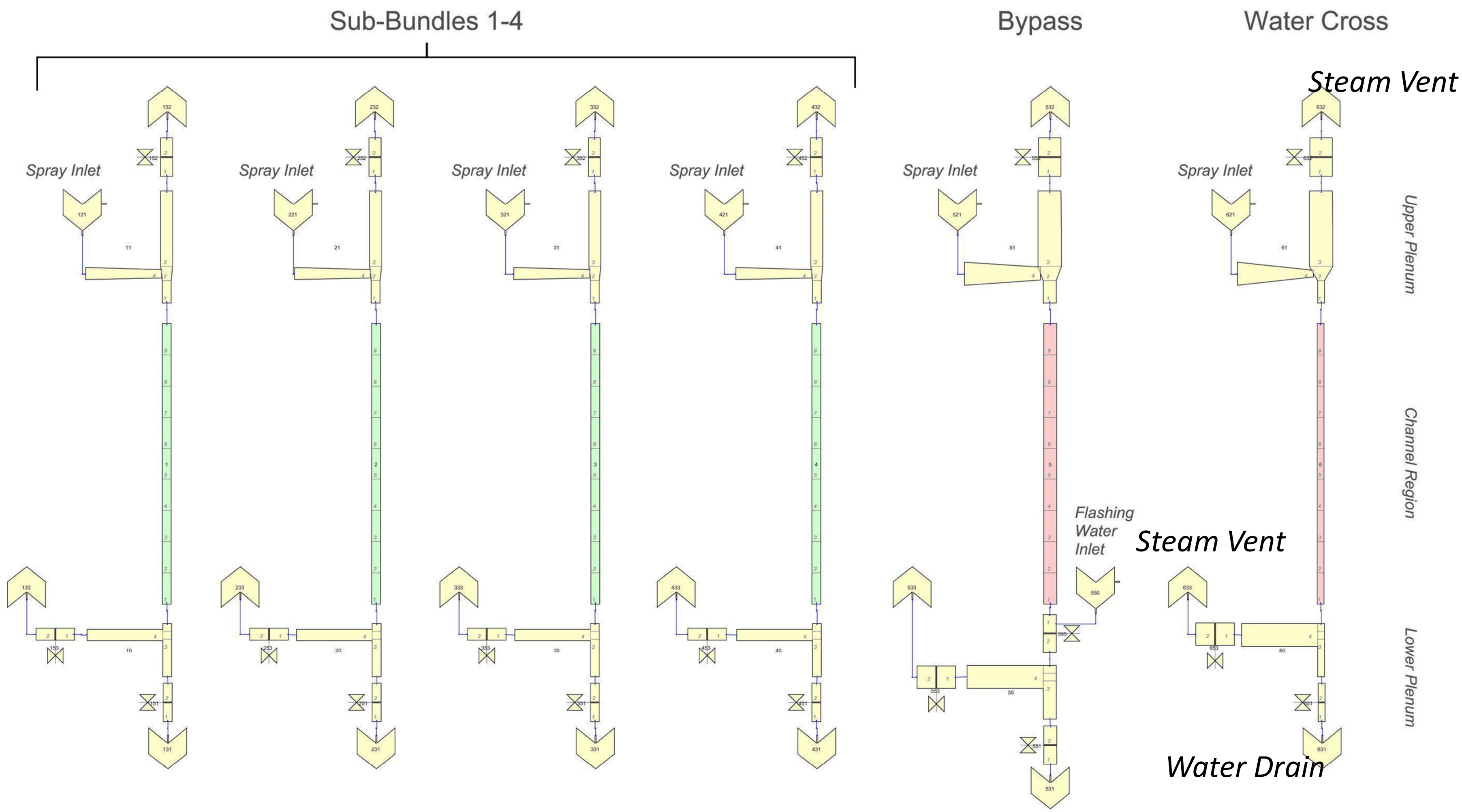
SVEA Spray Cooling Experiment



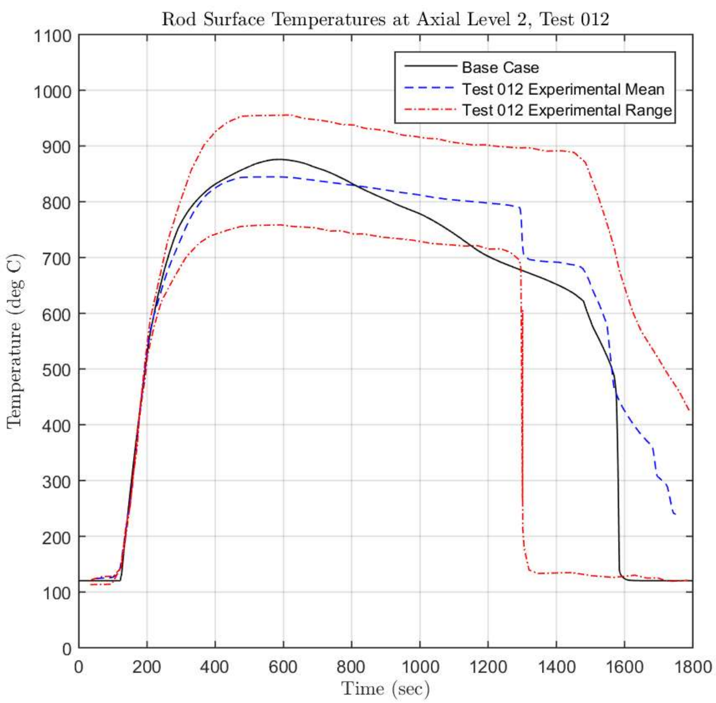


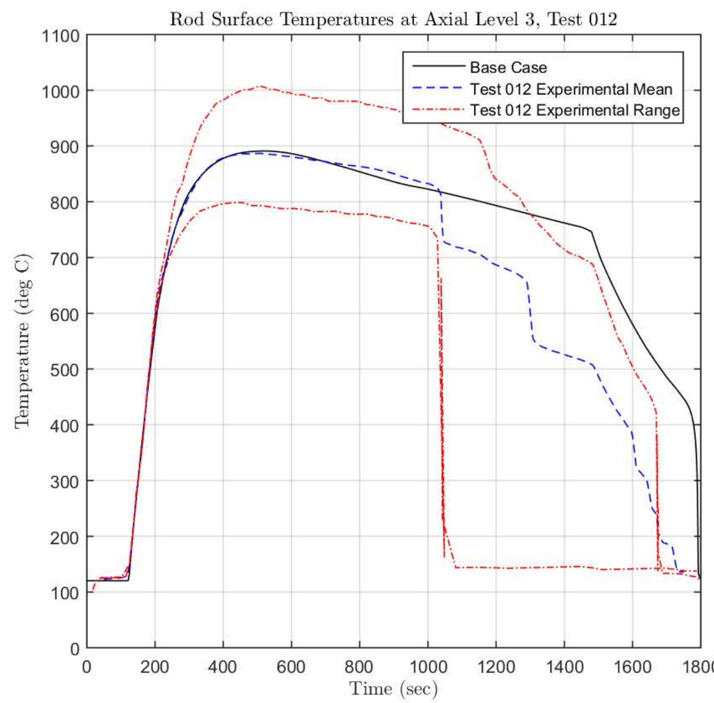


TRACE Model

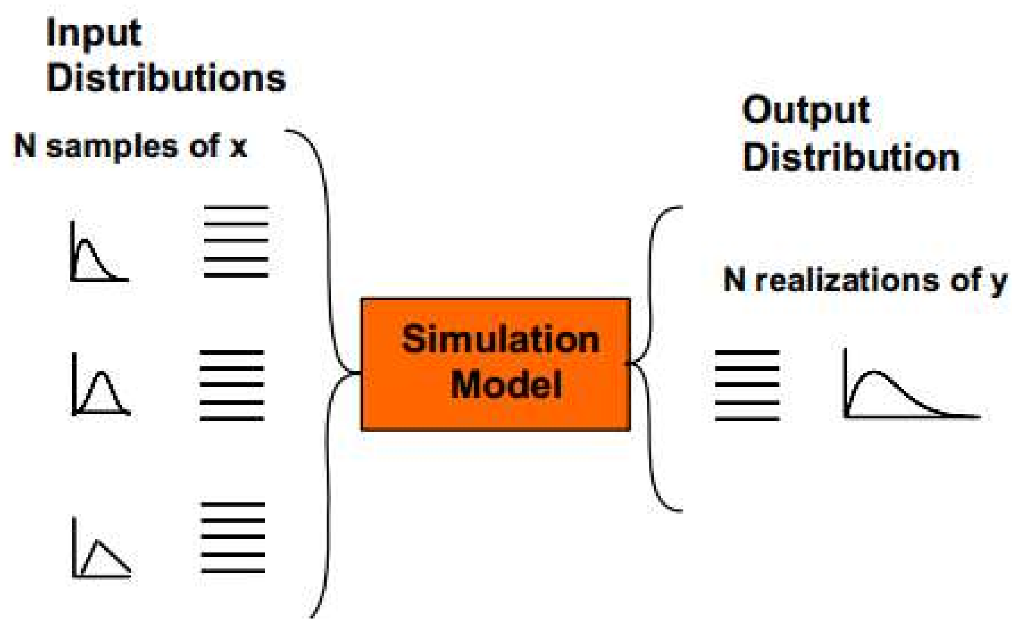

Sub-Bundles 1-4
Bypass
Water Cross
Steam Vent
Spray Inlet
Spray Inlet
Spray Inlet
Spray Inlet
Spray Inlet
Spray Inlet
Upper Plenum
Channel Region
Flashing Water Inlet
Steam Vent
Lower Plenum
Water Drain

Test 012 – Uniform spray (40 g/s)





Forward Uncertainty Quantification



Uncertainty Parameters, 1/4

No.	Parameter	Uncertainty	Reference Value
Thermal-Hydraulics Initial and Boundary Conditions			
1	Spray system pressure	0.1 bar	2 bar
2	Spray system temperature	0.75%	323 K
3	Bundle spray mass flow	1%	20-80 g/s
4	Bypass spray mass flow	1%	65-130 g/s
5	Water cross spray mass flow	1%	10 g/s
6	Water drain temperature	0.75%	323 K
7	Steam vent temperature	0.75%	393 K
8	Outlet pressure	0.1 bar	2 bar

Uncertainty Parameters, 2/4

No.	Parameter	Uncertainty	Reference Value
Vessel-related Parameters			
9	Bundle wall roughness	30%	1×10-6 m
10	Bypass channel wall roughness	30%	1×10-6 m
11	Water-cross wall roughness	30%	1×10-6 m
12	Length of main channel	0.01 m	3.68 m
13	Length of bypass channel	0.01 m	3.68 m
14	Length of water-cross	0.01 m	3.68 m

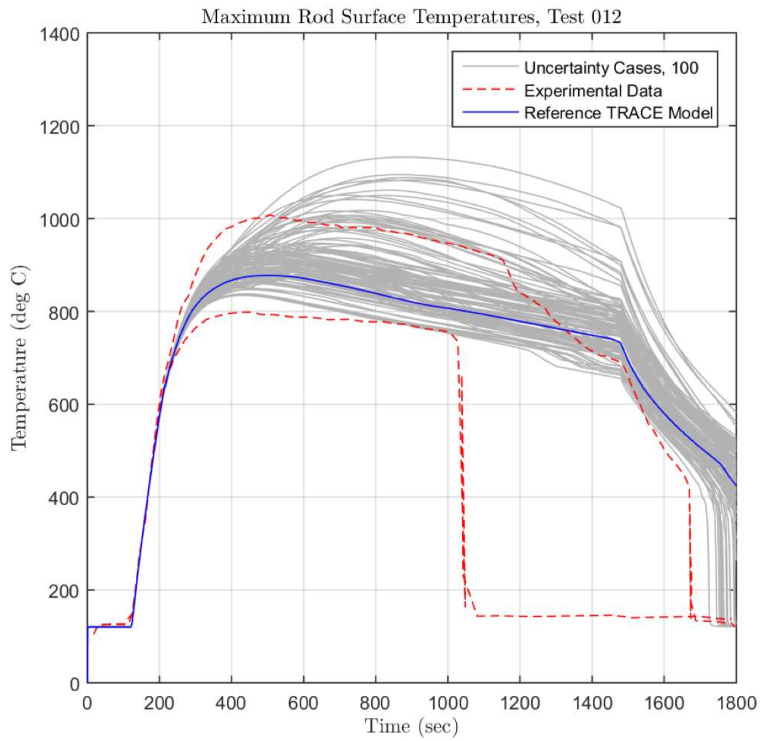
Uncertainty Parameters, 3/4

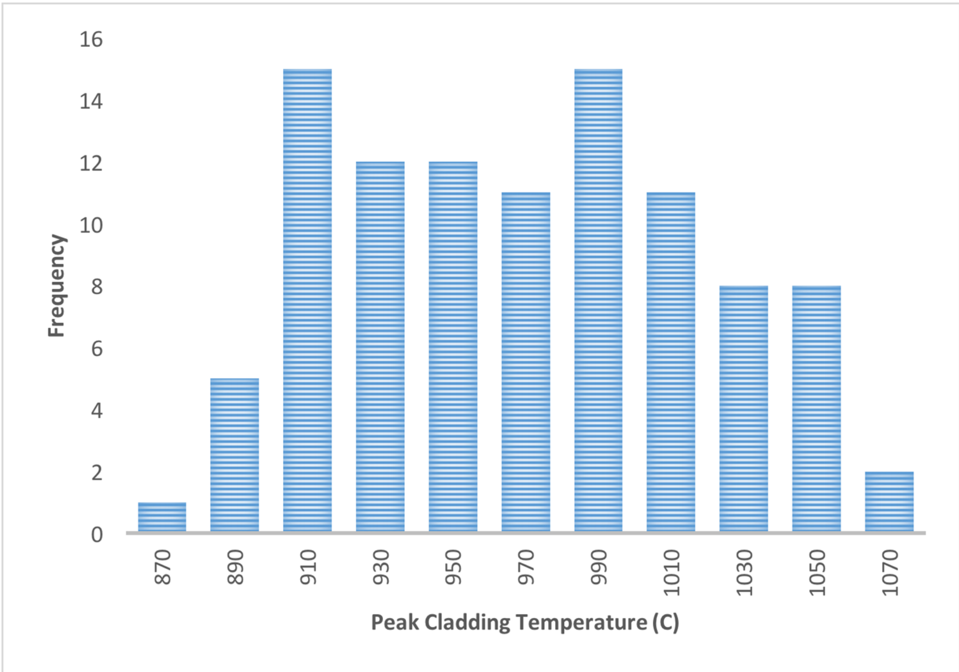
No.	Parameter	Uncertainty	Reference Value
Bundle-related Parameters			
15	Bundle flow area	1.00%	2.428×10-3 m2
16	Bundle hydraulic diameter	1.00%	0.01114 m
17	Bypass channel flow area	1.00%	6.14×10-3 m2
18	Bypass hydraulic diameter	1.00%	0.0884 m
19	Water Cross flow area	1.00%	1.612×10-3 m2
20	Water Cross hydraulic diameter	1.00%	0.0453 m
21	Rod emissivity	0.10	0.45
22	Bundle wall emissivity	0.10	0.3
23	CCFL slope	0.8-1.0	1.0
24	CCFL constant	0.88-1.0	1.0

Uncertainty Parameters, 4/4

No.	Parameter	Uncertainty	Reference Value
TRACE Physical Models – Heat Transfer			
25	DFFB Wall-Liquid HTC	45%	1.0
26	Wall Liquid HTC	15%	1.0
27	Wall Vapor HTC	20%	1.0
28	DNB/CHF	8%	1.0
TRACE Physical Models – Friction			
29	Annular-Mist Interfacial Drag	25%	1.0
30	DFFB Interfacial Drag	40%	1.0
31	Wall Drag	5%	1.0

DAKOTA simulation – 100 cases

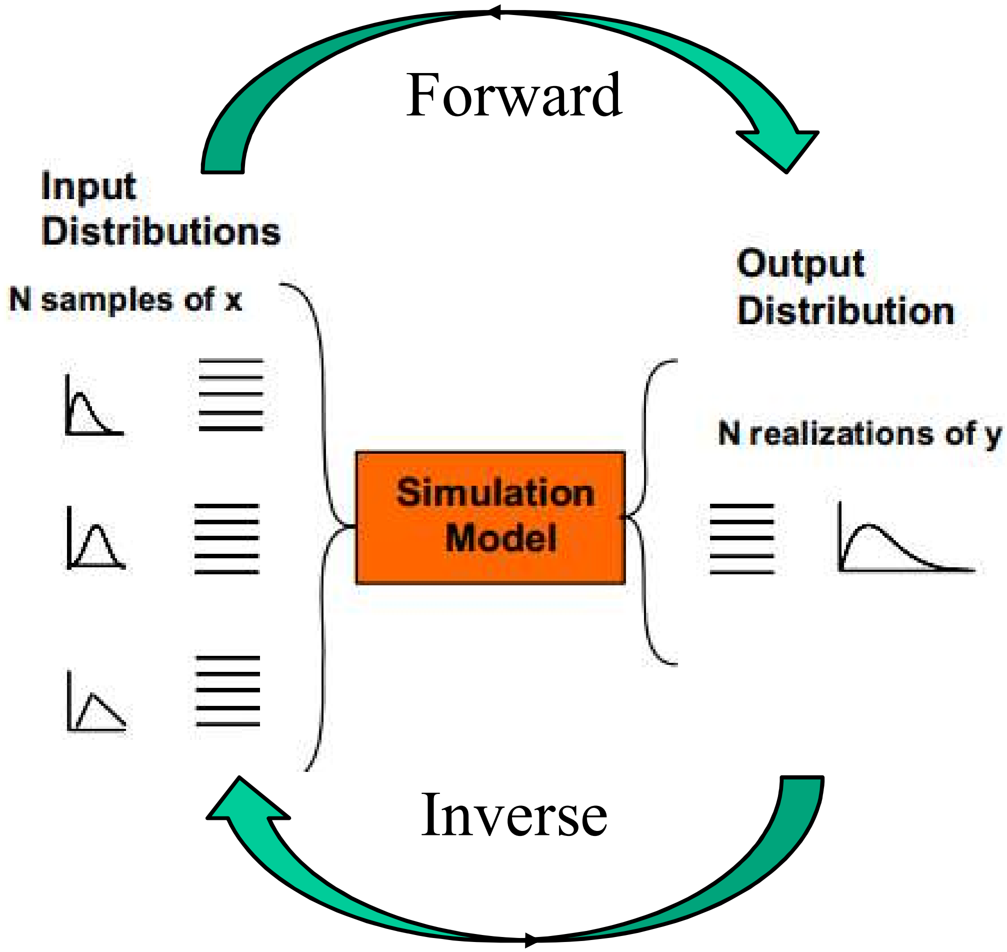




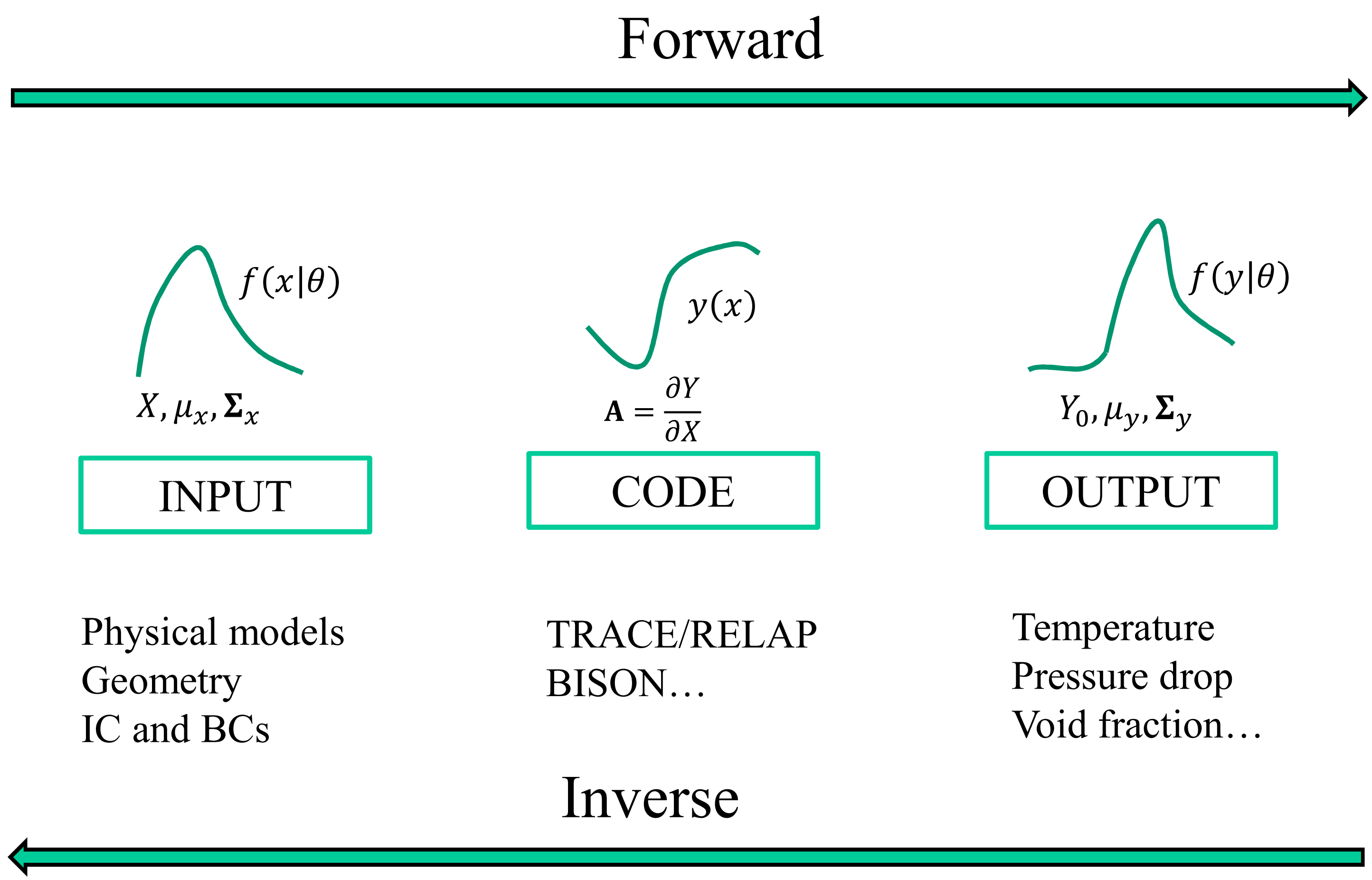
Uncertainty of Physical Models

No.	Parameter	Uncertainty	Reference Value
TRACE Physical Models – Heat Transfer			
25	DFFB Wall-Liquid HTC	**45%**	1.0
26	Wall Liquid HTC	**15%**	1.0
27	Wall Vapor HTC	**20%**	1.0
28	DNB/CHF	**8%**	1.0
TRACE Physical Models – Friction			
29	Annular-Mist Interfacial Drag	**25%**	1.0
30	DFFB Interfacial Drag	**40%**	1.0
31	Wall Drag	**5%**	1.0

Forward vs Inverse Uncertainty Quantification



Forward vs Inverse Uncertainty Quantification



Notations & Definitions

Meaning of variables

Variables	Meaning
$\vec{X}$	**input** model parameter random variable
$\vec{Y}$	**output** random variable from experimental **measurement**
$\vec{Y}_0$	**output** random variable from **code** prediction
$\vec{E}$	random **error** of experimental **measurement**
$\mathbf{A}$	**sensitivity coefficient** matrix
$\vec{\mu}_x, \mathbf{\Sigma}_x$	**mean** and **covariance** matrix of **input** model parameter random variable
$\vec{\mu}_y, \mathbf{\Sigma}_y$	**mean** and **covariance** matrix of **output** random variable
$\vec{\mu}_e, \mathbf{\Sigma}_e$	**mean** and **covariance** matrix of random **error** of experimental measurement
$\vec{\theta}$	parameter vector of the **mean** and **variance** of **input** model parameter

Notations & Definitions

- Likelihood $L(\vec{\theta}|x)$: The probability that observed x happens with parameter $\vec{\theta}$.

$$L(\vec{\theta}|x) \equiv f(x;\vec{\theta})$$

- Prior $\pi(\vec{\theta})$: Our prior knowledge about the parameters $\vec{\theta}$.
- Posterior $\pi(\vec{\theta}|x)$: Our updated knowledge about the parameter $\vec{\theta}$ after considering both the observed value x and prior knowledge.

$$\pi(\vec{\theta}|x) = \frac{L(\vec{\theta}|x)\pi(\vec{\theta})}{\int L(\vec{\theta}|x)\pi(\vec{\theta}))d\vec{\theta}} \equiv K(x)L(\vec{\theta}|x)\pi(\vec{\theta})$$

Assumptions

- $\vec{X}$ has a joint Gaussian distribution

$$f(\vec{x};\vec{\theta}) = \frac{1}{2\pi}|\mathbf{\Sigma}_x|^{-\frac{1}{2}}\exp[-\frac{1}{2}(\vec{x}-\vec{\mu}_x)^{\mathrm{T}}\mathbf{\Sigma}_x^{-1}(\vec{x}-\vec{\mu}_x)]$$

- $\delta\vec{Y}$ depends linearly on $\delta\vec{X}$ when $\delta\vec{X}$ is small

$$\vec{Y} = \vec{Y}_0 + \mathbf{A}\vec{X}$$

  where, the sensitivity coefficient matrix is obtained by,

$$\mathbf{A} = \frac{\boldsymbol{\partial}\vec{Y}}{\boldsymbol{\partial}\vec{X}}, \qquad \text{evaluated at nominal X}$$

  $\vec{Y}$ also follows joint Gaussian distribution, because of the linear relation.

- $\vec{E}$ is assumed to be mean-zero

$$\vec{Y} = \vec{Y}_0 + \mathbf{A}\vec{X} + \vec{E}$$

Likelihood function & Posterior distribution

Suppose there are $i = 1, 2, \ldots, N$ sets of observed data (or experiments), we assume $\vec{Y}_i$'s are independent to each other. Then we have,

$$\vec{Y}_i = \vec{Y}_{0,i} + \mathbf{A}_i \vec{X} + \vec{E}_i$$

$$f_i(\vec{y};\vec{\theta}) = \frac{1}{2\pi} |\mathbf{\Sigma}_{y,i}|^{-\frac{\mathrm{dy}}{2}} \exp[-\frac{1}{2}(\vec{y} - \vec{\mu}_{y,i})^{\mathrm{T}} \mathbf{\Sigma}_{y,i}^{-1} (\vec{y} - \vec{\mu}_{y,i})]$$

with,

$$\vec{\mu}_{y,i} = \vec{Y}_{0,i} + \mathbf{A}_i \vec{\mu}_x$$

$$\mathbf{\Sigma}_{y,i} = \mathbf{A}_i \mathbf{\Sigma}_x \mathbf{A}_i^{\mathrm{T}} + \mathbf{\Sigma}_{e,i}$$

The likelihood function $L(\vec{\theta}|\mathbf{y})$ and posterior distribution $\pi(\vec{\theta}|\mathbf{y})$ is,

$$L(\vec{\theta}|\mathbf{y}) = \prod_{i=1}^{N} \frac{1}{2\pi} |\mathbf{\Sigma}_{y,i}|^{-\frac{\mathrm{dy}}{2}} \exp[-\frac{1}{2}(\vec{y}_i - \vec{\mu}_{y,i})^{\mathrm{T}} \mathbf{\Sigma}_{y,i}^{-1} (\vec{y}_i - \vec{\mu}_{y,i})]$$

$$\pi(\vec{\theta}|\mathbf{y}) = K(\mathbf{y})\pi(\vec{\theta}) \prod_{i=1}^{N} \frac{1}{2\pi} |\mathbf{\Sigma}_{y,i}|^{-\frac{\mathrm{dy}}{2}} \exp[-\frac{1}{2}(\vec{y}_i - \vec{\mu}_{y,i})^{\mathrm{T}} \mathbf{\Sigma}_{y,i}^{-1} (\vec{y}_i - \vec{\mu}_{y,i})]$$

Notes: The likelihood function and posterior distribution are the base for following MLE, MAP and MCMC algorithm.

MLE

Idea: maximize the likelihood function to solve for parameter vector $\vec{\theta}$

E-M algorithm:

- Maximization. With $\mathbf{\Sigma}_x$ known, $\vec{u}_{x,\text{new}}$ is solved by maximizing the Log-likelihood function.

$$\vec{u}_{x,\text{new}} = \max_{\vec{u}_x} \log L(\vec{\theta}|\mathbf{y})$$

with the Log-likelihood function,

$$\log L(\vec{\theta}|\mathbf{y}) = \sum_{i=1}^{N} [-\frac{\mathrm{d_y}}{2}\log|\mathbf{\Sigma}_{y,i}| - \log 2\pi - \frac{1}{2}(\vec{y}_i - \vec{\mu}_{y,i})^{\mathrm{T}}\mathbf{\Sigma}_{y,i}^{-1}(\vec{y}_i - \vec{\mu}_{y,i})]$$

- Expectation. With $\vec{u}_{x,\text{new}}$ known, $\mathbf{\Sigma}_x$ is updated using conditional expectation.

$$\mathbf{\Sigma}_{x,\text{new}} = \mathrm{E}[(\vec{X} - \vec{u}_{x,\text{new}})(\vec{X} - \vec{u}_{x,\text{new}})^{\mathrm{T}}|\mathbf{y}]$$

MLE: E-M algorithm

- Maximization step (update mean value)

Let the derivative of the log-likelihood function with respect to $\vec{\mu}_x$ to be zero,

$$\frac{\partial \log L(\vec{\theta}|\mathbf{y})}{\partial \vec{\mu}_x} = \frac{\partial \sum_{i=1}^{N} [-\frac{\mathrm{d_y}}{2}\log|\boldsymbol{\Sigma}_{y,i}| - \log 2\pi - \frac{1}{2}(\vec{y}_i - \vec{\mu}_{y,i})^{\mathrm{T}}\boldsymbol{\Sigma}_{y,i}^{-1}(\vec{y}_i - \vec{\mu}_{y,i})]}{\partial \vec{\mu}_x} = 0$$

We get the equation to update mean value,

$$\left(\sum_{i=1}^{N} \mathbf{A}_i^{\mathrm{T}}\boldsymbol{\Sigma}_{y,i}^{-1}\mathbf{A}_i\right)\vec{\mu}_{x,\mathrm{new}} = \sum_{i=1}^{N} \mathbf{A}_i^{\mathrm{T}}\boldsymbol{\Sigma}_{y,i}^{-1}(\vec{y}_i - \vec{y}_{0,i})$$

- Expectation step (update covariance)

After the mean value $\vec{\mu}_x$ has been updated, the covariance matrix is updated by:

$$\boldsymbol{\Sigma}_{x,\mathrm{new}} = \mathrm{E}[(\vec{X} - \vec{u}_{x,\mathrm{new}})(\vec{X} - \vec{u}_{x,\mathrm{new}})^{\mathrm{T}}|\mathbf{y}]$$

$$= \boldsymbol{\Sigma}_{x,\mathrm{old}} + \frac{1}{N}\sum_{i=1}^{N} \left(-\boldsymbol{\Sigma}_{xy,i}^{\mathrm{T}}\boldsymbol{\Sigma}_{y,i}^{-1}\boldsymbol{\Sigma}_{xy,i} + [\boldsymbol{\Sigma}_{xy,i}^{\mathrm{T}}\boldsymbol{\Sigma}_{y,i}^{-1}(\vec{y}_i - \vec{\mu}_{y,i})][\boldsymbol{\Sigma}_{xy,i}^{\mathrm{T}}\boldsymbol{\Sigma}_{y,i}^{-1}(\vec{y}_i - \vec{\mu}_{y,i})]^{\mathrm{T}}\right)$$

where $\boldsymbol{\Sigma}_{xy,i}$ is correlation matrix,

$$\boldsymbol{\Sigma}_{xy,i} = \mathrm{cov}(\vec{X}, \vec{Y}_i) = \mathbf{A}_i\boldsymbol{\Sigma}_x$$

MAP

Idea: maximize the posterior distribution to solve for the parameter vector $\vec{\theta}$

Difference with MLE: prior distribution $\pi(\vec{\theta})$ and constant $K(\mathbf{y})$

$$\pi(\vec{\theta}|\mathbf{y}) = K(\mathbf{y})\pi(\vec{\theta}) \prod_{i=1}^{N} \frac{1}{2\pi} |\boldsymbol{\Sigma}_{y,i}|^{-\frac{\mathrm{dy}}{2}} \exp[-\frac{1}{2}(\vec{y}_i - \vec{\mu}_{y,i})^{\mathrm{T}} \boldsymbol{\Sigma}_{y,i}^{-1} (\vec{y}_i - \vec{\mu}_{y,i})]$$

- Maximization step needs considering prior distribution effect,

$$\left(\sum_{i=1}^{N} \mathbf{A}_i^{\mathrm{T}} \boldsymbol{\Sigma}_{y,i}^{-1} \mathbf{A}_i + \mathbf{M}_{\pi}\right) \vec{\mu}_{x,\mathrm{new}} = \sum_{i=1}^{N} \mathbf{A}_i^{\mathrm{T}} \boldsymbol{\Sigma}_{y,i}^{-1} \left(\vec{y}_i - \vec{y}_{0,i}\right) + \vec{\mathrm{B}}_{\pi}$$

  $\mathbf{M}_{\pi}$ and $\vec{B}_{\pi}$ depends on the prior distribution in practical application.

- Expectation step is the same as MLE.

Recall: $\pi(\vec{\theta}|x) = \frac{L(\vec{\theta}|x)\pi(\vec{\theta})}{\int L(\vec{\theta}|x)\pi(\vec{\theta}))d\vec{\theta}} \equiv K(x)L(\vec{\theta}|x)\pi(\vec{\theta})$

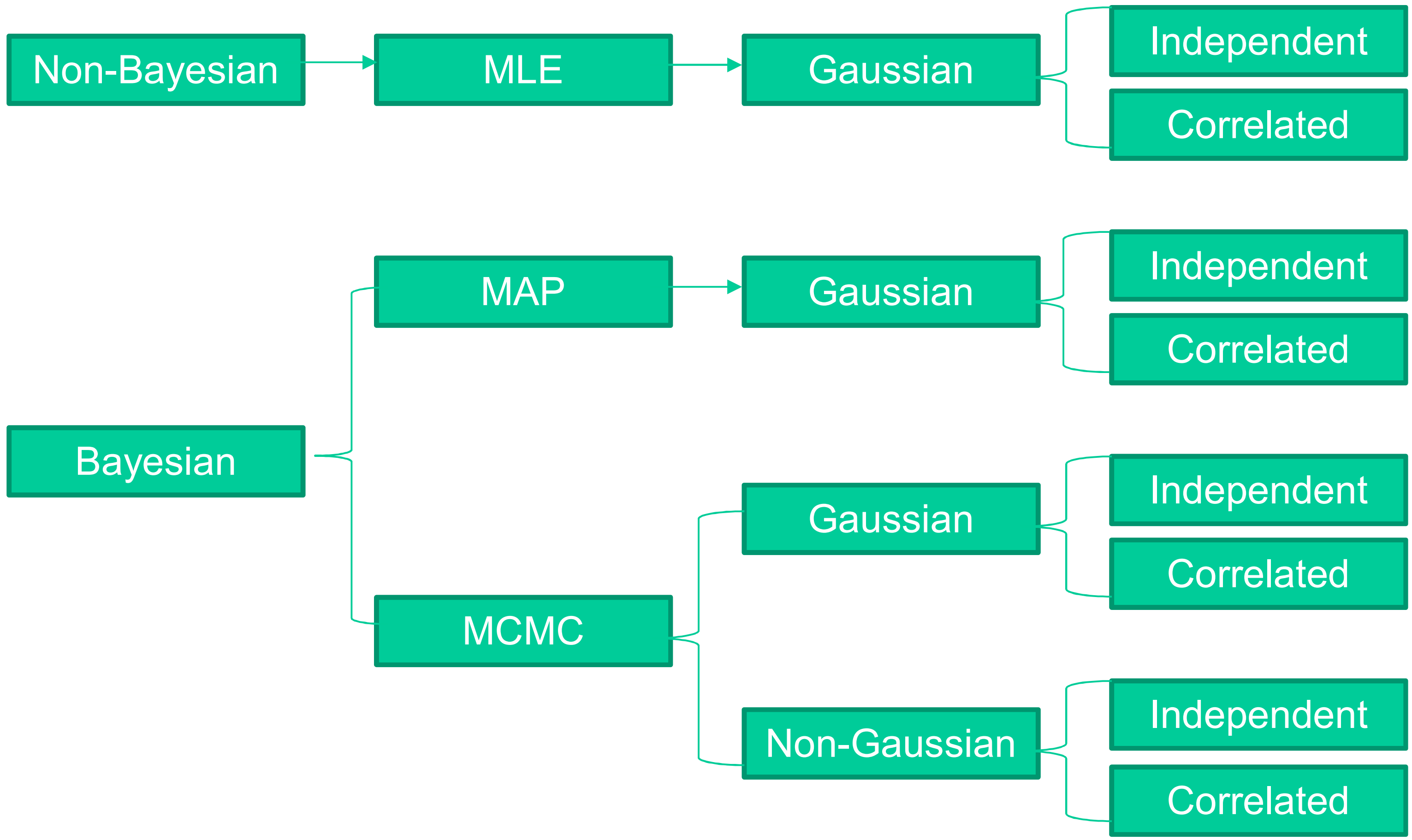
MCMC

Problems with MLE and MAP

- $L(\vec{\theta}|\mathbf{y})$. Maximization of likelihood function is difficult for distribution other than Gaussian distribution.
- $\pi(\vec{\theta})$. Should be differentiable to be used in MAP algorithm.
- $K(\mathbf{y})$. Has to be obtained with a multi-dimensional integration.

MCMC: sample the posterior distribution without performing the integration for $K(\mathbf{y})$. This sampling is implemented by using an iterative Monte Carlo sampling, which usually forms a Markov Chain.

Inverse Methods for Parameter Estimation

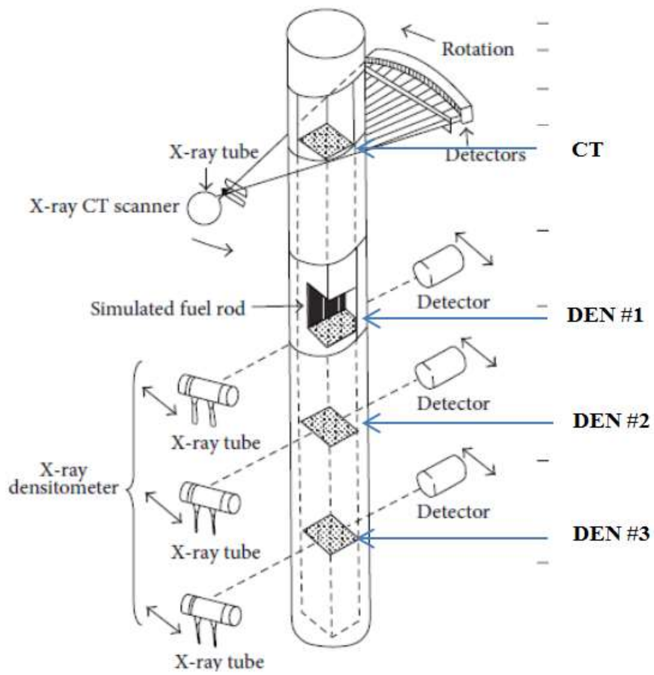


Distinguished by statistical methods

Distinguished by distribution of $\vec{X}$

Application: BFBT introduction

BFBT benchmark: The BFBT benchmark is a valuable benchmark for the sub-channel analysis of two-phase flow in BWR rod bundles.



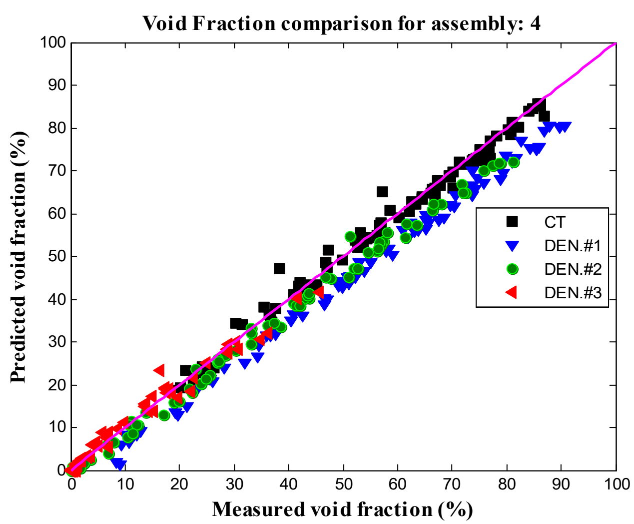
Parameters	**Variations**
Pressure (MPa)	3.9 - 8.7
Inlet temperature (°C)	238 - 292
Inlet subcooling (kJ/kg)	50. - 56.
Flow rate (t/h)	10. - 70.
Power (MW)	0.62 - 7.3
Exit quality (%)	8 - 25
Exit void fraction (%)	45 - 90

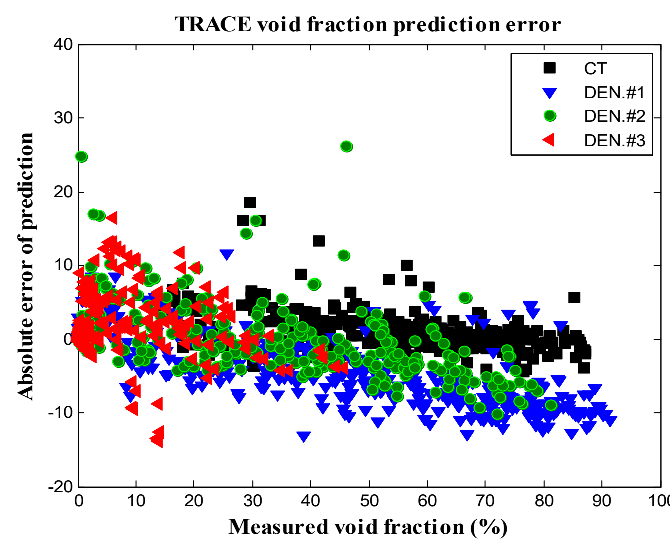
Application: analysis steps

1. Accuracy analysis: compare TRACE predictions with measurements. ($\vec{Y}_0$, $\vec{Y}$, $\vec{E}$)
2. Sensitivity analysis: obtain sensitivity coefficient matrix using TRACE. ($\mathbf{A}$)
3. Linearity assumption validation. ($\mathbf{A}$)
4. Inverse uncertainty quantification: estimate with MLE, MAP and MCMC. ($\vec{\mu}_x, \mathbf{\Sigma}_x$)
5. Validate MLE, MAP and MCMC results. ($\vec{\mu}_x, \mathbf{\Sigma}_x$)

Step 1: Accuracy analysis of TRACE prediction

TRACE void fraction predictions: at 4 axial elevations, and compared with the experimental measurement data.





Step 2: Sensitivity analysis of model parameters

Sensitivity coefficient: approximated with TRACE using finite difference method

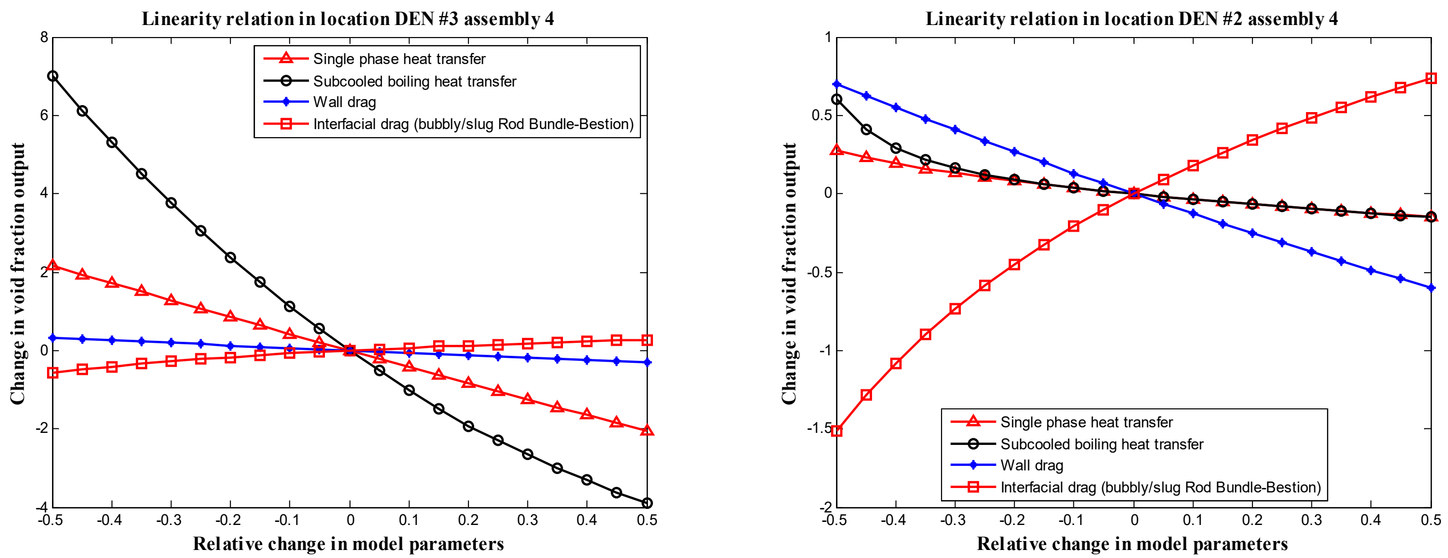
Parameters	DEN #3	DEN #2	DEN #1	CT
Single phase liquid to wall heat transfer	-4.22	-0.36	-0.20	-0.03
Subcooled boiling heat transfer	-10.77	-0.38	-0.20	-0.03
Wall drag	-0.63	-1.28	-1.66	-2.97
Interfacial drag (bubbly/slug rod rundle-Bestion)	0.73	1.94	2.25	0.93

Sensitivity coefficient = $\frac{\Delta Y}{\Delta X}\frac{X}{Y} * 100\%$

Step 3: Linearity assumption validation

Approach: obtain $\vec{Y}(\vec{X})$ using TRACE

Result: linearity assumption is valid in the relative range [-0.5, 0.5]



Step 4: Inverse uncertainty quantification

Criterion for selecting data:

1. The measured void fraction should be positive.
2. The predicted void fraction should be positive.
3. The absolute value of sensitivity coefficient should be larger than a pre-set tolerance (0.1).

Prior distribution:

- Conjugate prior distribution for MAP

Variables	Meaning	Value
$\vec{r}$	shape factor of normal-inverse gamma distribution	$(3,3)^T$
$\vec{k}$	shape factor of normal-inverse gamma distribution	$(1.0,1.0)^T$
$\vec{\beta}$	expectation value of prior $\vec{\mu}$	$(1.0,1.0)^T$
$\vec{\lambda}$	expectation value of prior $\vec{\sigma}^2$	$(1.0,1.0)^T$

- Prior distribution for MCMC

Algorithms	Prior type	Prior distribution
MCMC 1	**Non-informative**	$\frac{1}{(\sigma^1)^2(\sigma^2)^2}$
MCMC 2	**Conjugate**	previous Table
MCMC 3	**Uniform**	$\vec{\mu} \in [0.5,1.5] \times [0.5,1.5]$, $\vec{\sigma}^2 \in [0.,1.0] \times [0.,1.0]$

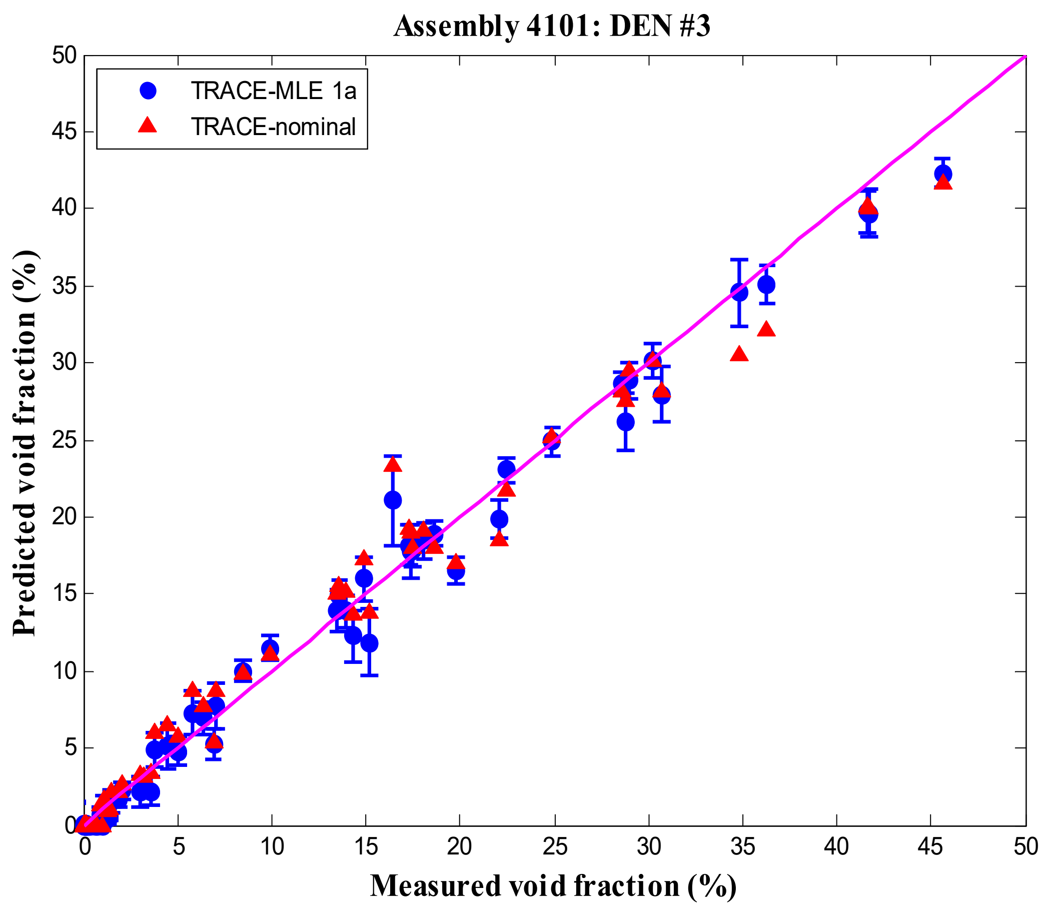
Step 4: IUQ with MLE, MAP, MCMC

Compare results

- MLE results: information from data
- MLE vs MCMC 1: very close, because non-informative prior does not provide prior information
- MLE vs MAP, MCMC 2 and MCMC 3: the results are weighted by prior information.

Algorithms	**Subcooled boiling HTC**	**Interfacial drag(bubbly/slug)**	**Correlation**
MLE	1.15 ± 0.05	1.70 ± 0.17	0.31
MAP	1.06 ± 0.21	1.24 ± 0.46	0.16
MCMC 1	1.15 ± 0.05	1.69 ± 0.21	N/A
MCMC 2	1.11 ± 0.29	1.46 ± 0.52	N/A
MCMC 3	1.11 ± 0.12	1.32 ± 0.50	N/A

Step 5: Forward uncertainty propagation (validation of inverse uncertainty)



Conclusions

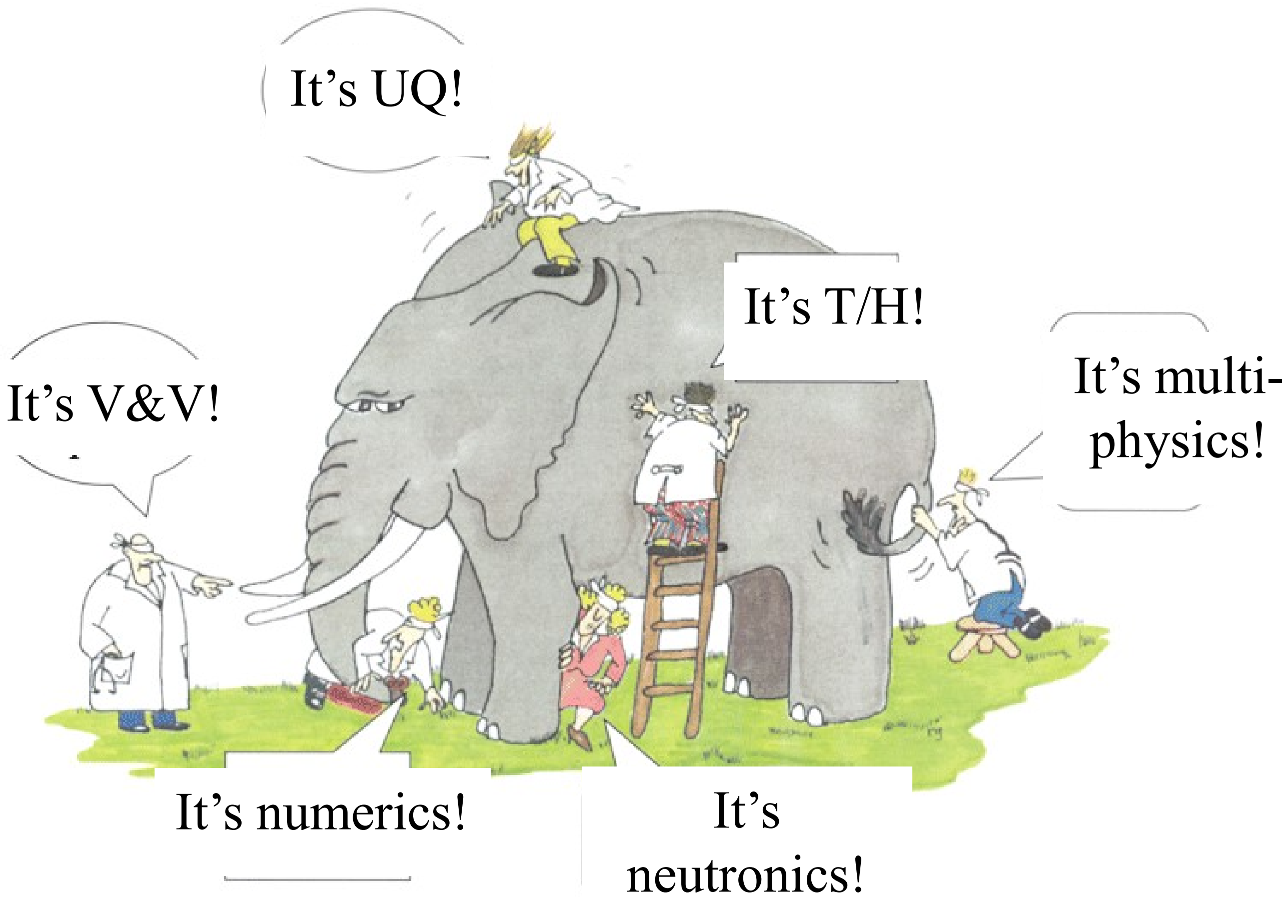
- Quantification of uncertainties of **input physical models** is possible
  - No need to guess input model uncertainty, no need of expert judgment
  - But methodology cannot be used as black box

- Facilitates in subsequent forward UQ endeavors

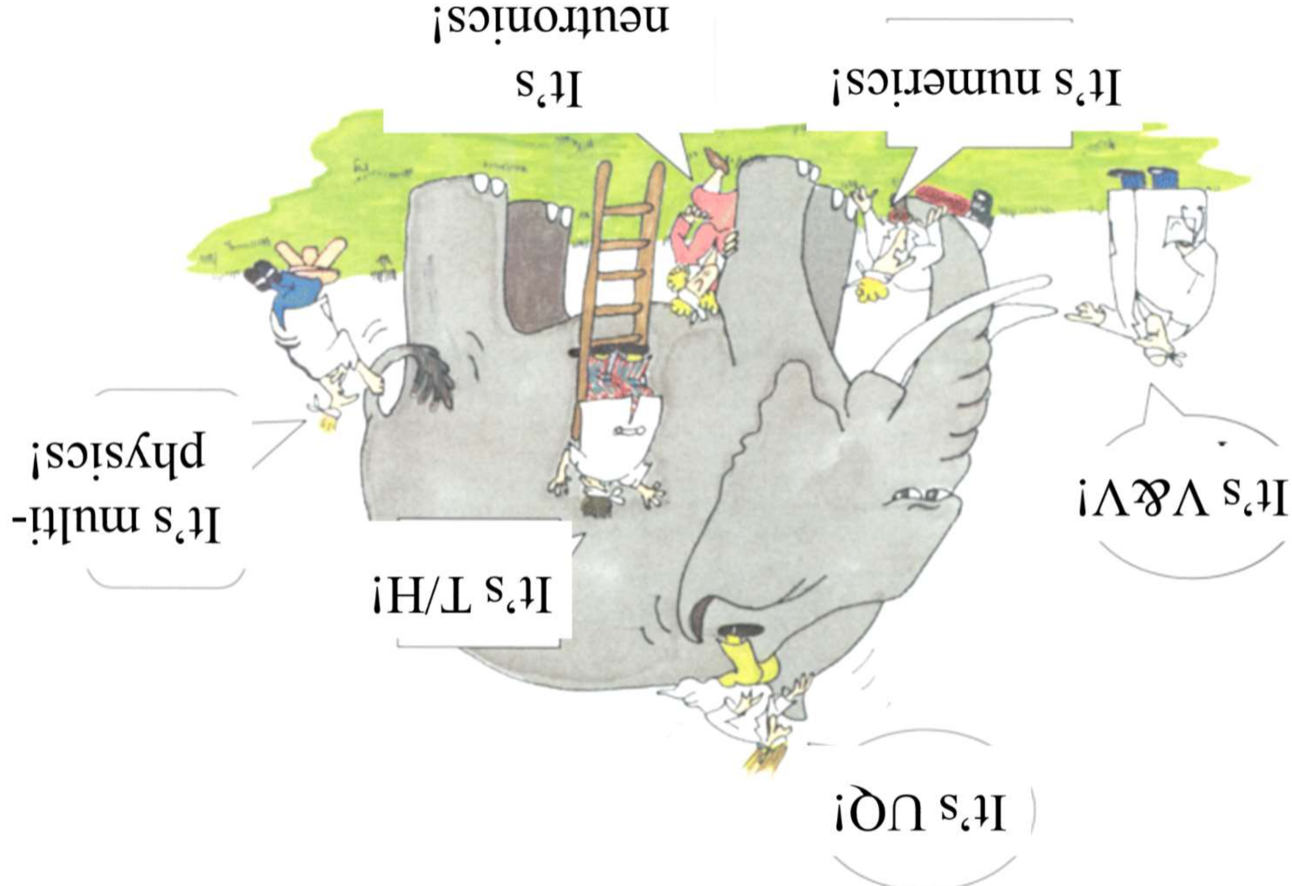
- Challenges
  - Prior information: we should provide appropriate prior distribution. If not, use MLE instead.
  - Linearity assumption between input and output: use high-order surrogate model

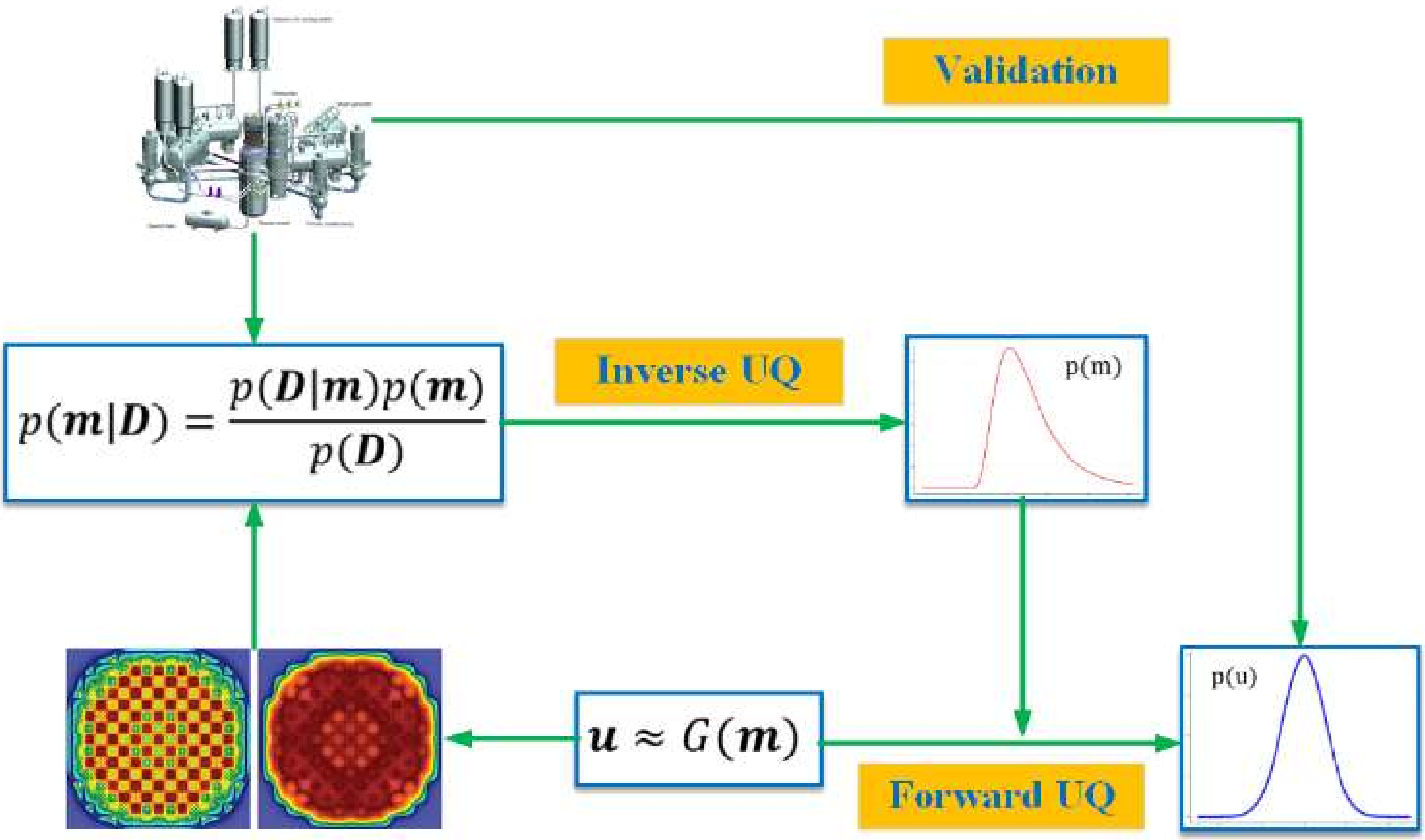
- **Additional application**
  - **Extendible to other system/codes (RELAP5, MELCOR, BISON, …)**
  - **Extendible to other fields: insurance, finance, operations research, …**

So what was it all about?



So what was it all about?




Validation
p(m|D) = p(D|m)p(m) / p(D)
Inverse UQ
p(m)
p(u)
u ≈ G(m)
Forward UQ

Forward vs Inverse Uncertainty Quantification