An approach to evaluate uncertainties in complex CFD simulations

Romain CAMY
romain.camy@edf.fr

Research Engineer
EDF R&D

November 2013

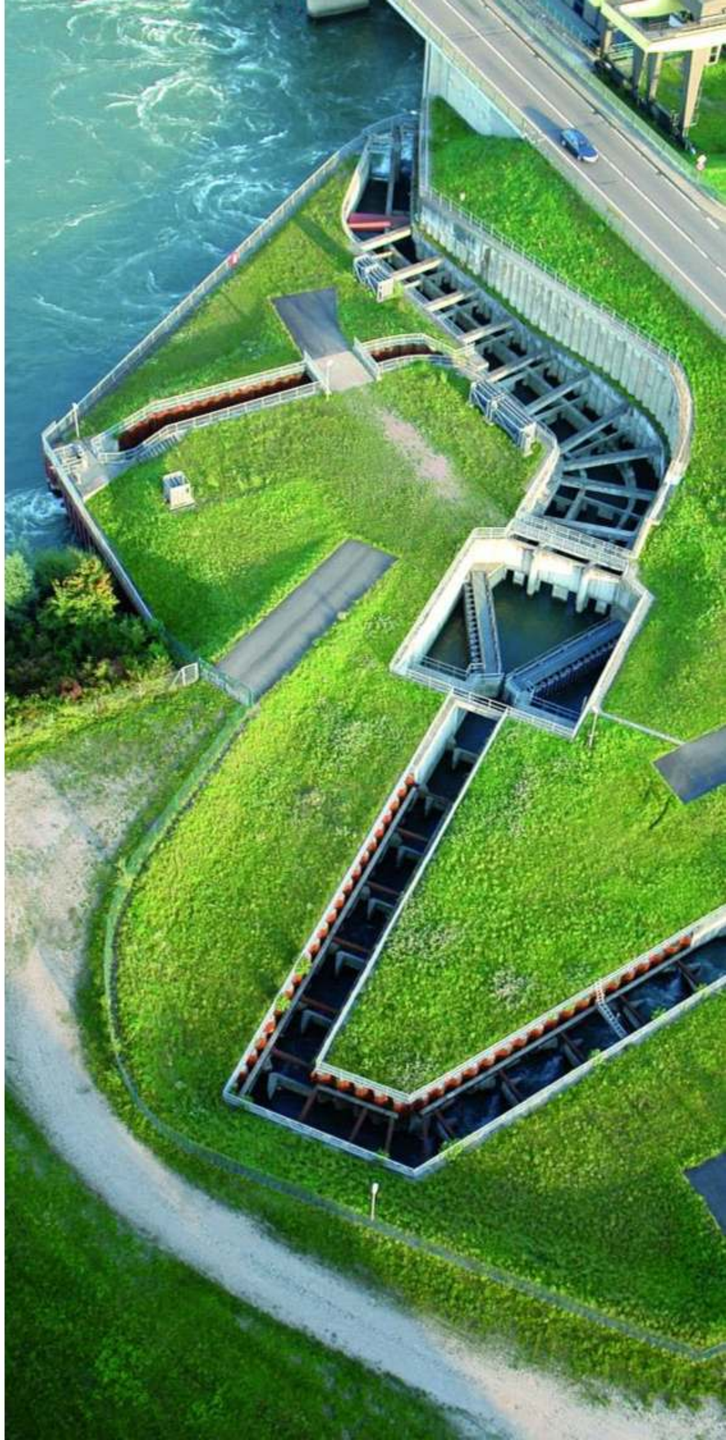


Table of content

1. A practical example
2. A chaotic industrial flow example
3. A pragmatic approach (ICARE)
4. Step-by-step description of the procedure
5. Results in an actual R&D nuclear study
6. Conclusions and short term prospects

A practical example

- We consider a simple physical phenomenon: the crushing load y of a given mechanical part made of a given material as a function of its thickness x.

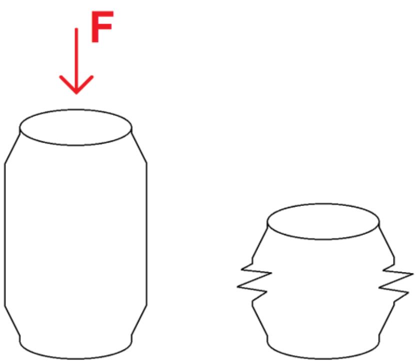
$$y = f(x)$$

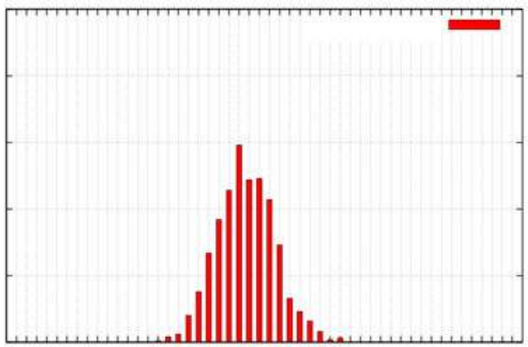
- What is expected (implicitly most of the time):

$$\lim_{\varepsilon \to 0} f(x + \varepsilon) = f(x)$$

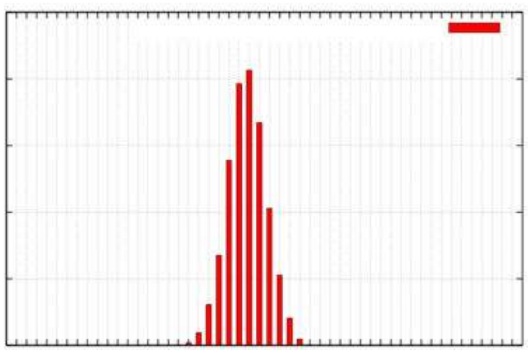
A practical example

- If we do the experiment with for example soda cans. We measure wall thickness and record the load y=F when it crushes → big dispersion for small variations of thickness.





- Further, if we select cans with the same thickness (according to our measurements) we will still get a significant dispersion.



A practical example

- What happened here is that at our macroscopic scale, identical cans exhibit different crushing load. It seems that:

$$\lim_{\varepsilon \to 0} f(x+\varepsilon) \neq f(x)$$

- Reasons are:
  - Cans are actually not identical
  - Physical equations are strongly non linear

- Consequences if you had to calculate how many cans can be stacked one over the other for transportation: you would have uncertainty on that number even if at your macroscopic scale, there is no uncertainty on cans material, thickness and so on.

- Unfortunately, fluid mechanics equations are also strongly non linear.

- Fortunately, uncertainties propagation takes necessarily this extra uncertainty source into account.

A chaotic industrial flow example

- Objective: Assess thermal load uncertainties in a Pressurized Thermal Shock (PTS) transient following a Loss Of Coolant Accident (LOCA).

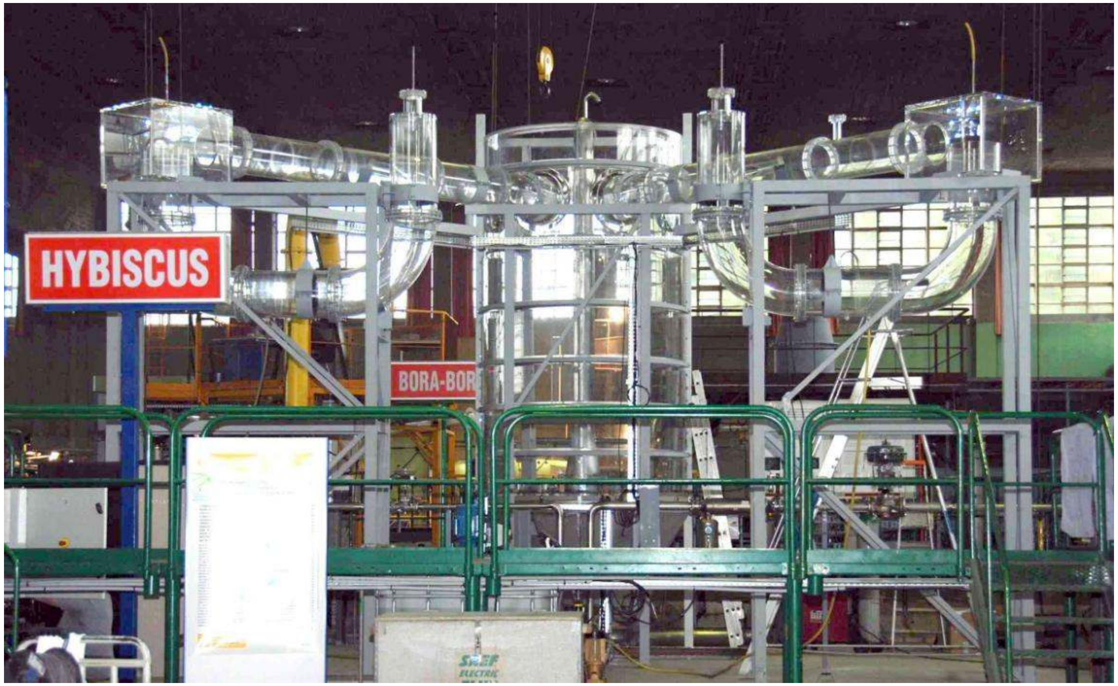
- At EDF R&D Chatou, we develop an open source Computational Fluid Dynamics (CFD) code. *Code_Saturne* (http://code-saturne.org).

CODE SATURNE

- Numerical PWR PTS transient (simulation with *Code_Saturne*):
  - REP_ICARE_x5.avi

A chaotic industrial flow example

- At EDF R&D Chatou, we also operate a 0.5 scale mock-up of a Pressurized Water Reactor (PWR) primary loop (experimental setup about 5m high):



- Experimental HYBISCUS II test case:
  - HII_ICARE_exp.avi
- Numerical HYBISCUS II test case (simulation with *Code_Saturne*):
  - HII_ICARE.avi

A pragmatic approach (ICARE)

- 9 Sources of uncertainties identified
  1. Approximate physical models
  2. Discretisation error
  3. Convergence error
  4. Round-off errors
  5. Error in geometry definition
  6. Domain limitation error
  7. Oversight of influencing physical phenomena
  8. Uncertain input physical parameters
  9. Error arising from chaotic behaviour

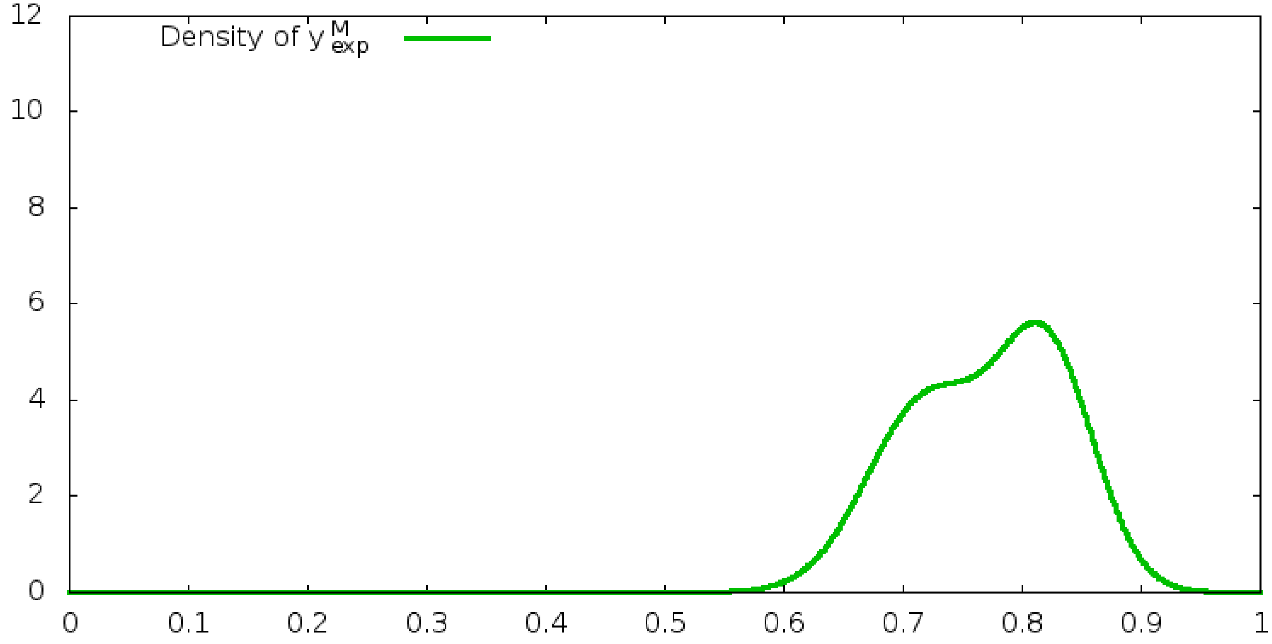
- Dealing with all of them is intractable in complex simulations → rely on experimental data from integral validation[1] experimental test cases to estimate 7 first points.

[1] integral validation experimental test case : Means a test case that is for a certain physics fully representative of the considered full scale device.

Step-by-step description of the procedure

- We consider an integral validation experiment repeated n_{exp} times.

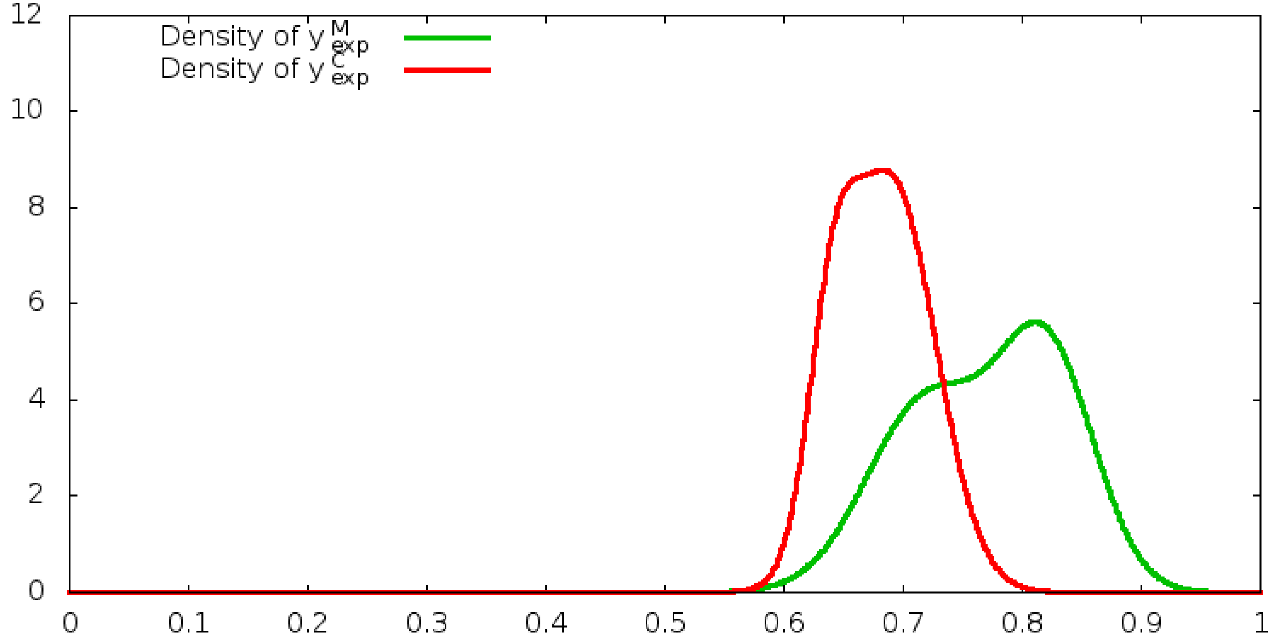
- We consider the n_{exp} measures of these n_{exp} experiments (here and after, measure is supposed to be reality). If the experiments have chaotic features, one will get significant dispersion for very similar conditions $\underline{x}^{M}_{exp,i}$, i ϵ [1, n_{exp}].



Step-by-step description of the procedure

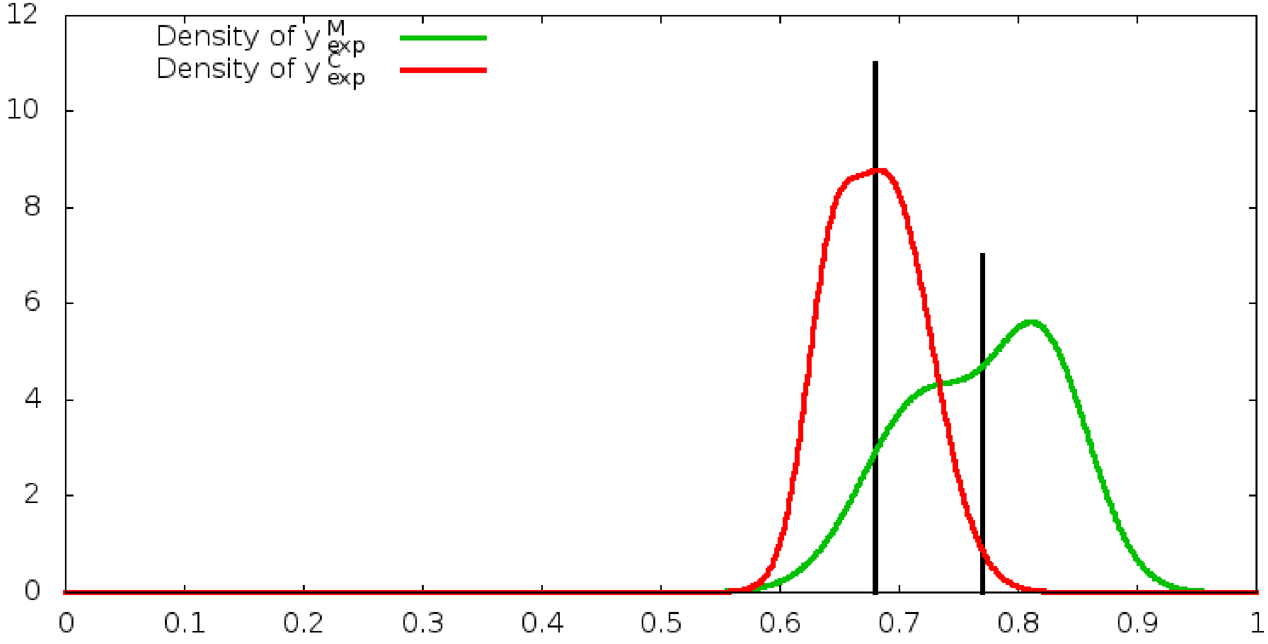
- We make n_{exp} calculations with our Model and the n_{exp} sets of measured experimental conditions $\underline{x}^M_{exp,i}$. Each calculation corresponds to a particular experimental run.

- If physics is chaotic, the calculations have to reproduce this behavior and lead to a dispersion comparable to the one of measures.



Step-by-step description of the procedure

- We calculate mean values for both measured and calculated results.

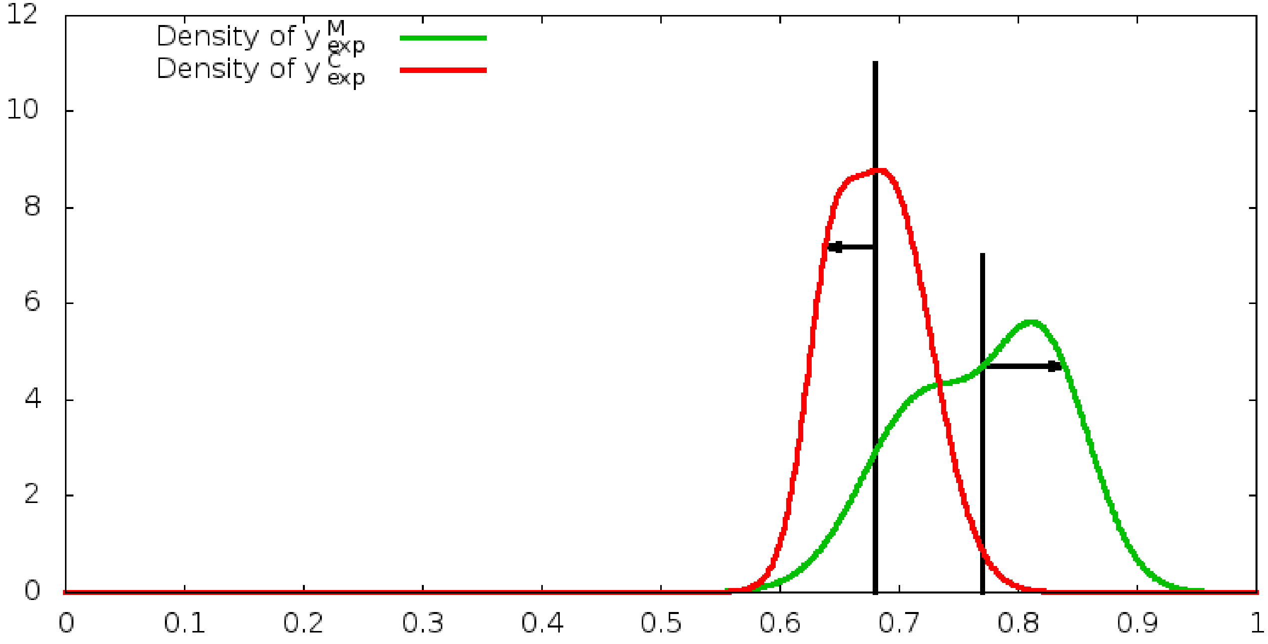


Step-by-step description of the procedure

- We calculate standard deviations for both measured and calculated results.

- We quantify Model error by considering ratios of mean values and standard deviations:

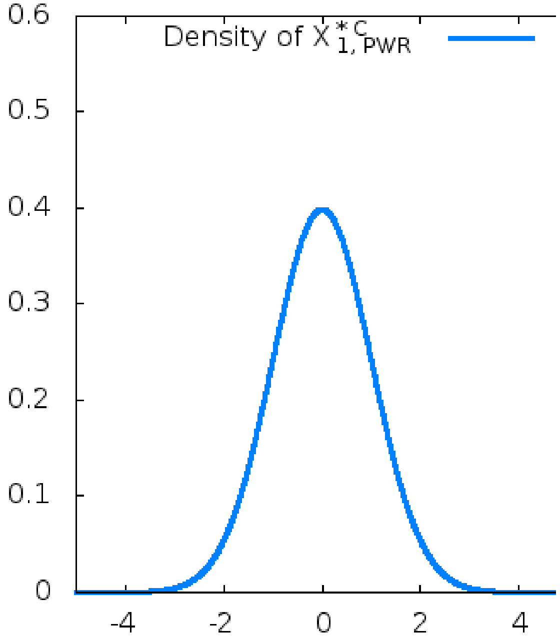
$$\frac{\mu^{\mathrm{M}}_{\mathrm{exp}}}{\mu^{\mathrm{C}}_{\mathrm{exp}}}, \frac{\sigma^{\mathrm{M}}_{\mathrm{exp}}}{\sigma^{\mathrm{C}}_{\mathrm{exp}}}$$

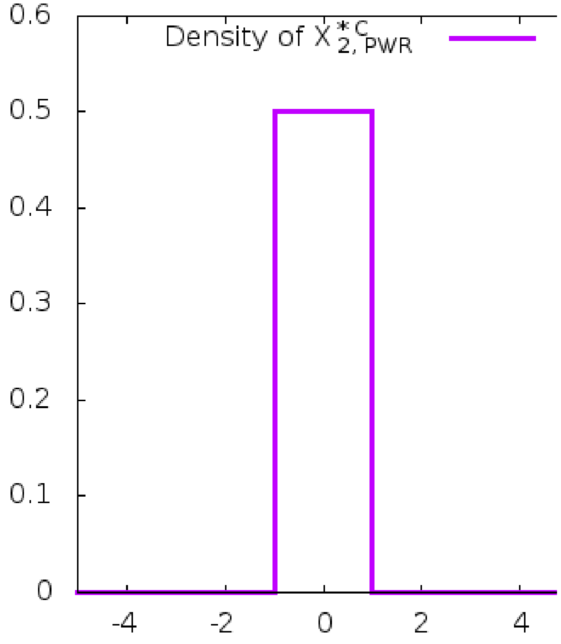


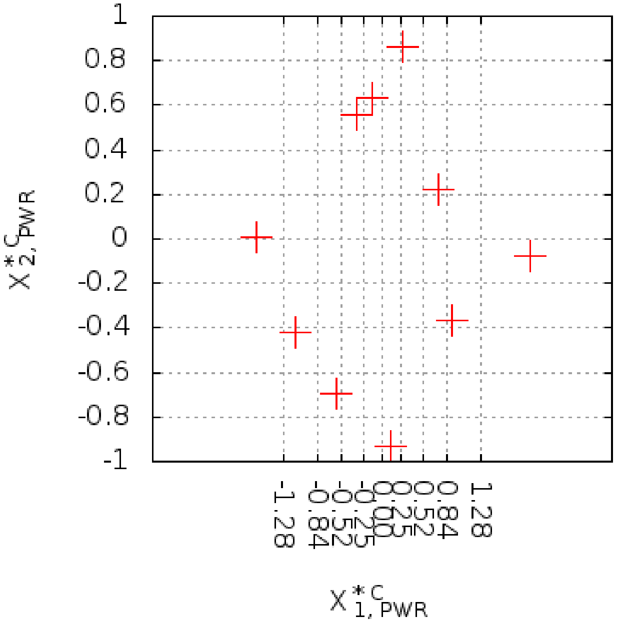
Step-by-step description of the procedure

- We consider our Model at industrial scale case. The industrial and test case Models have to be similar (similar characteristic length, similar non dimensional numbers and similar non dimensional results).

- We consider uncertain input parameters of the Model used at industrial scale and create a Design Of Experiments (DOE) of n_{PWR} points accordingly.

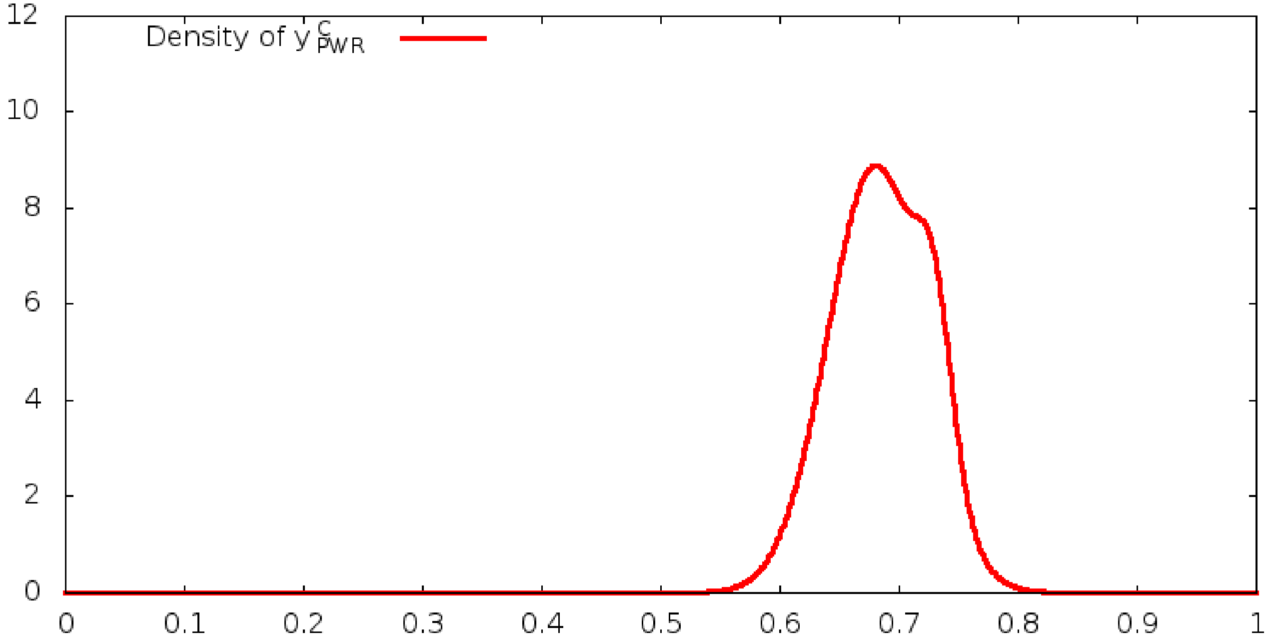






Step-by-step description of the procedure

- Propagation of uncertainties gives n_{PWR} calculation results (we have no measures at industrial scale) having a dispersion due to:
  - significant variations in the input ;
  - inherent variability of the physics.

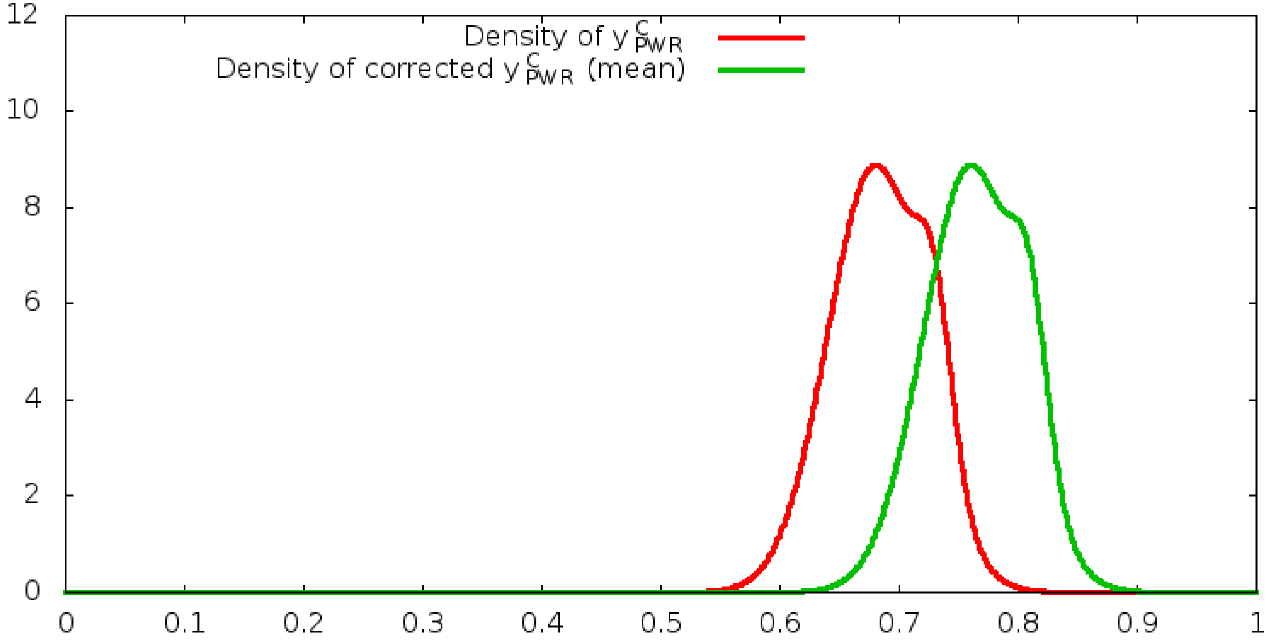


Step-by-step description of the procedure

- We can correct each calculation result with the tendency, observed at test case scale, to under- / over- estimate average value:

$$\varphi(y_{\mathrm{PWR}}^{\mathrm{C}}) = y_{\mathrm{PWR}}^{\mathrm{C}} \frac{\mu_{\mathrm{exp}}^{\mathrm{M}}}{\mu_{\mathrm{exp}}^{\mathrm{C}}}$$

- Geometrically, it results in a translation of the density.



Step-by-step description of the procedure

- To correct each calculation result with the tendency, observed at test case scale, to under- / over- estimate inherent variability of the results we need to isolate at industrial scale inherent variability from variability due to significant variations of input parameters.

- This separation requires an estimation of the expectancy of y^C_{PWR} conditional to $\underline{x}^C_{PWR}$. It can be done with a regression and a least square estimation of the coefficients, for example:

$$\mu^{\mathrm{C}}_{\mathrm{PWR}}(\underline{x}^{\mathrm{C}}_{\mathrm{PWR}}) = \sum_{j=1}^{n_x} a_j x_j + a_0$$

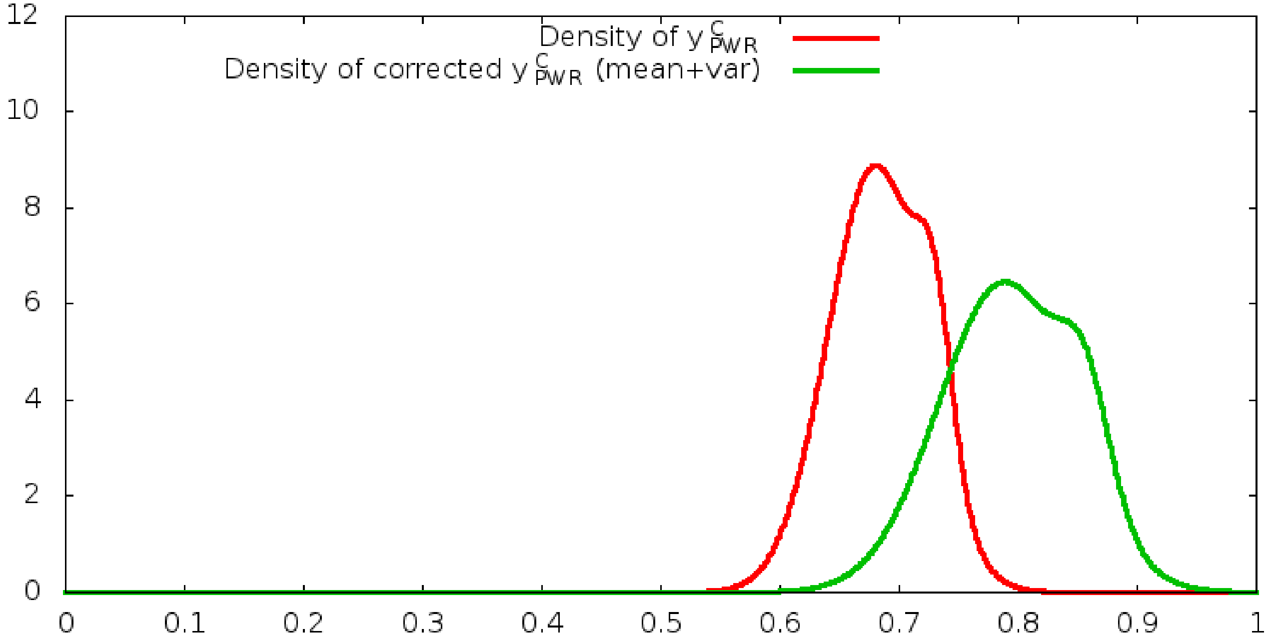
$$\mu^{\mathrm{C}}_{\mathrm{PWR}}(\underline{x}^{\mathrm{C}}_{\mathrm{PWR}}) = \arg\min_{\underline{x}^{\mathrm{C}}_{\mathrm{PWR}}} \left\{ \sum_{i=1}^{n^{\mathrm{C}}_{\mathrm{PWR}}} \left[y^{\mathrm{C}}_{\mathrm{PWR}} - \mu^{\mathrm{C}}_{\mathrm{PWR}}(\underline{x}^{\mathrm{C}}_{\mathrm{PWR,\ i}}) \right]^2 \right\}$$

Step-by-step description of the procedure

- Once this term calculated, it is possible to corect each Model result with, also, the tendency, observed at test case scale, to under- / over- estimate inherent variability of the results:

$$\varphi(y^{\mathrm{C}}_{\mathrm{PWR}}) = [y^{\mathrm{C}}_{\mathrm{PWR}} - \mu^{\mathrm{C}}_{\mathrm{PWR}}]\frac{\sigma^{\mathrm{M}}_{\mathrm{exp}}}{\sigma^{\mathrm{C}}_{\mathrm{exp}}} + \mu^{\mathrm{C}}_{\mathrm{PWR}}\frac{\mu^{\mathrm{M}}_{\mathrm{exp}}}{\mu^{\mathrm{C}}_{\mathrm{exp}}}$$

- Geometrically, it results in a contraction/dilatation of the density.



Step-by-step description of the procedure

- When dealing with results function of time, the procedure can be repeated at each time step. The same can be done for a function of space at each discrete position.

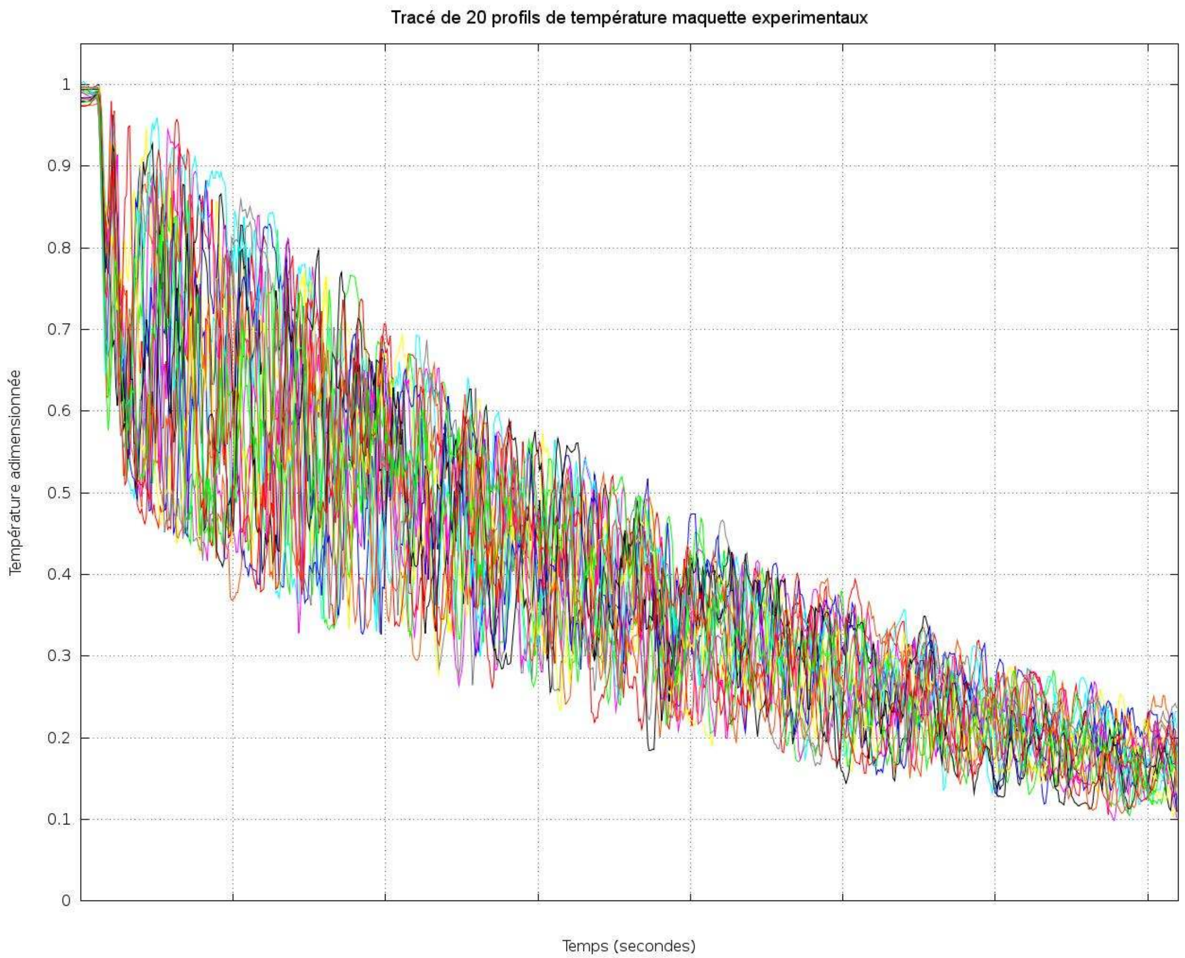
- Final results take into account:
  - Model flaws observed at test case scale ;
  - Variability due to uncertain input parameters and chaotic behavior.

- In the end, it is possible to have an estimate of the impact of each source of uncertainty (chaos and uncertain input parameters separated) on calculation results.

- Also, if transposition of errors from test case scale to industrial scale is hard to justify one can still use the piece of information: *"if my Model exhibits the same errors at industrial scale and test case scale then the impact on the results is x%"* .

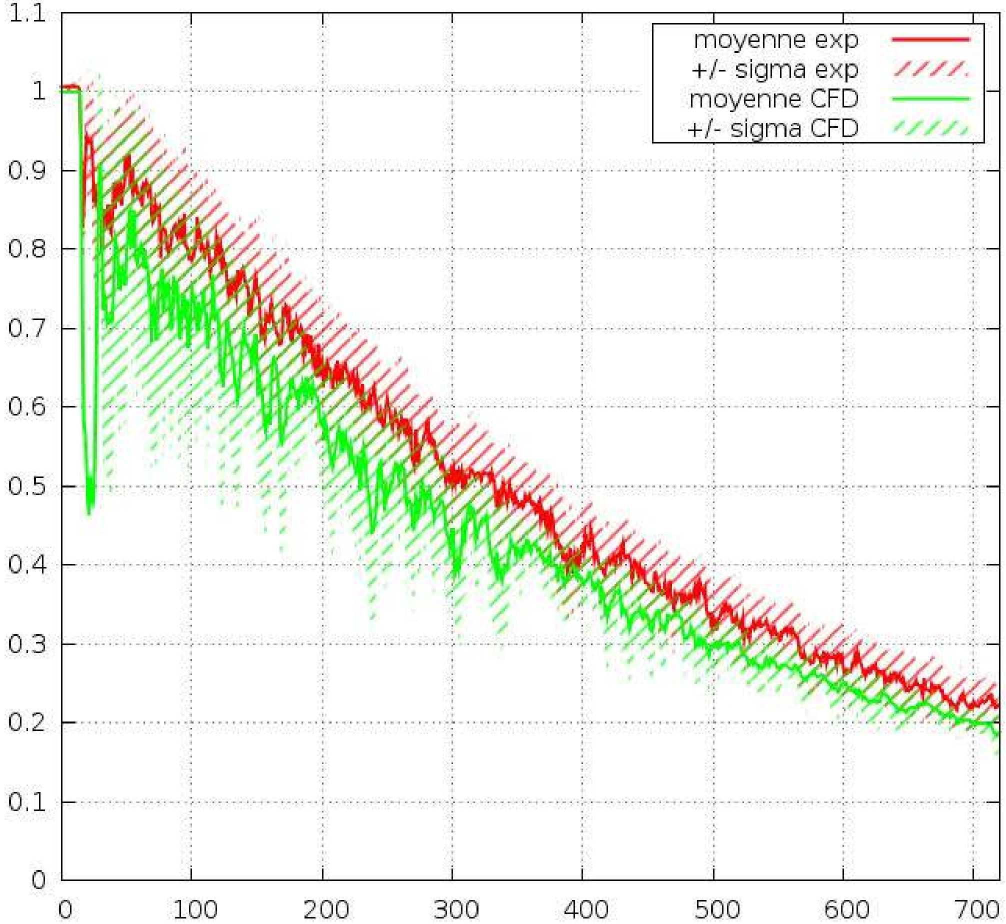
Results in an actual R&D nuclear study

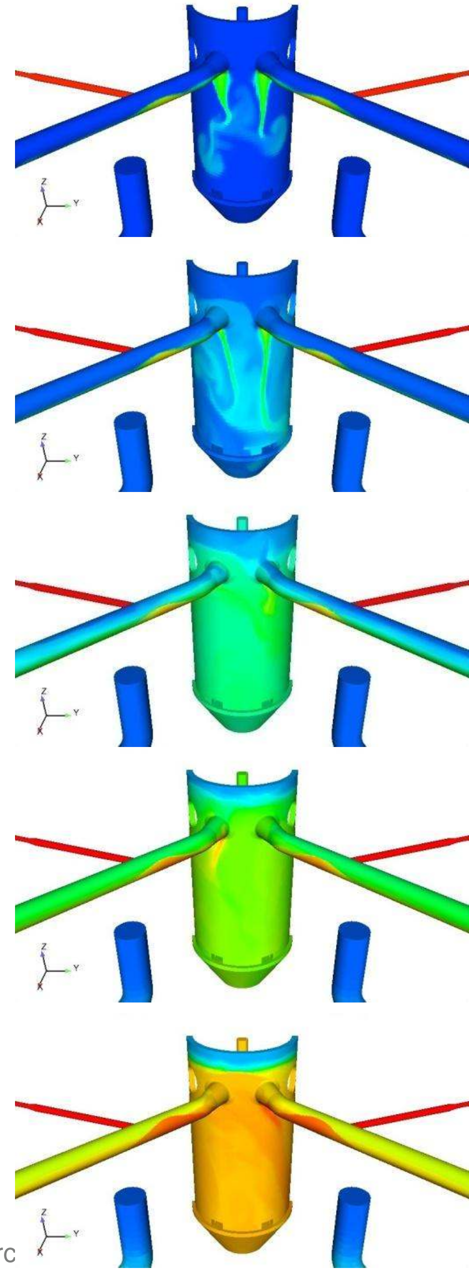
- Here are 20 temperature profiles obtained at a given location for repeated experiments on HYBISCUS II:



Results in an actual R&D nuclear study

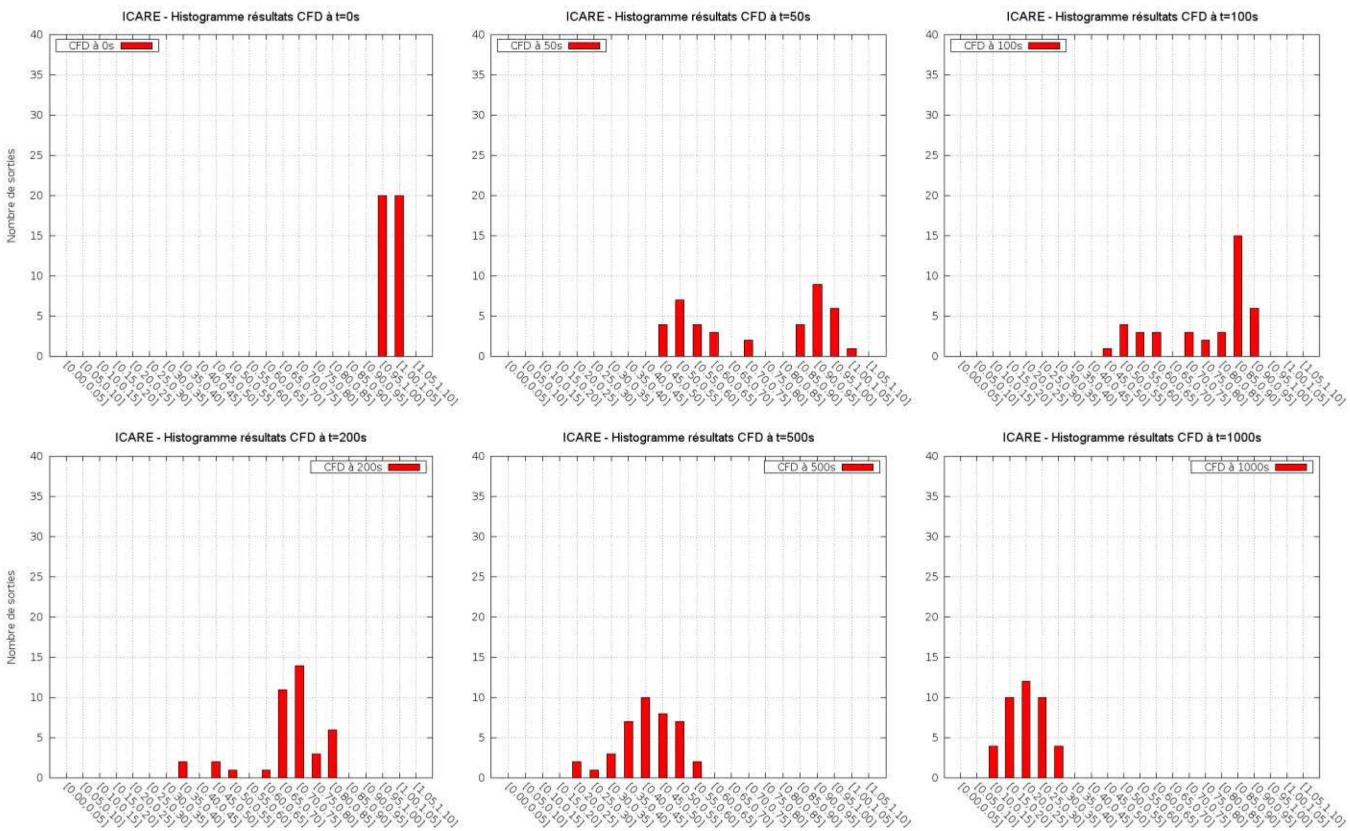
- At this location, comparison with 20 CFD results by mean and variance gives:

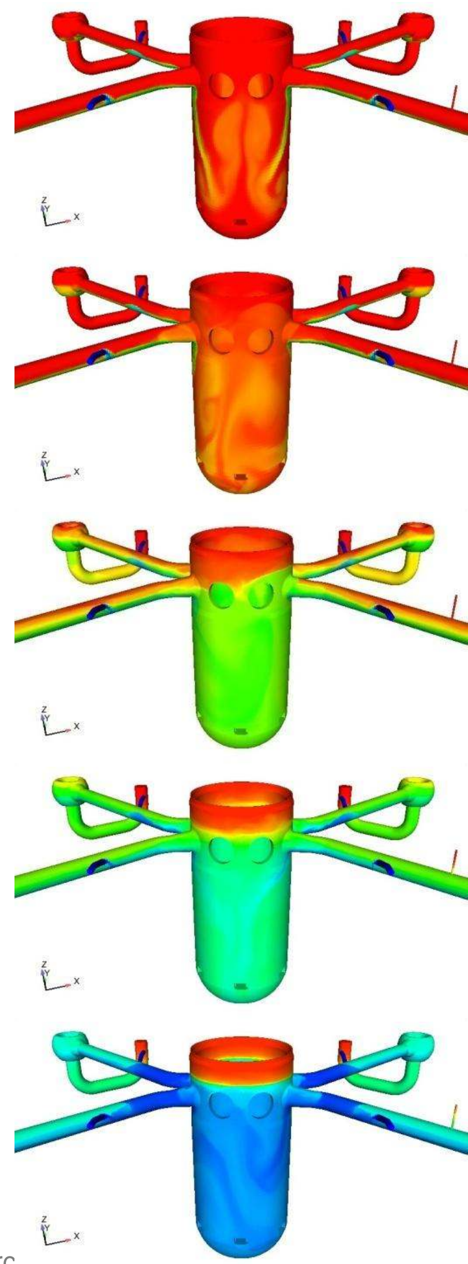




Results in an actual R&D nuclear study

- Here are 40 CFD results (bar charts only used for visualization) at different times:

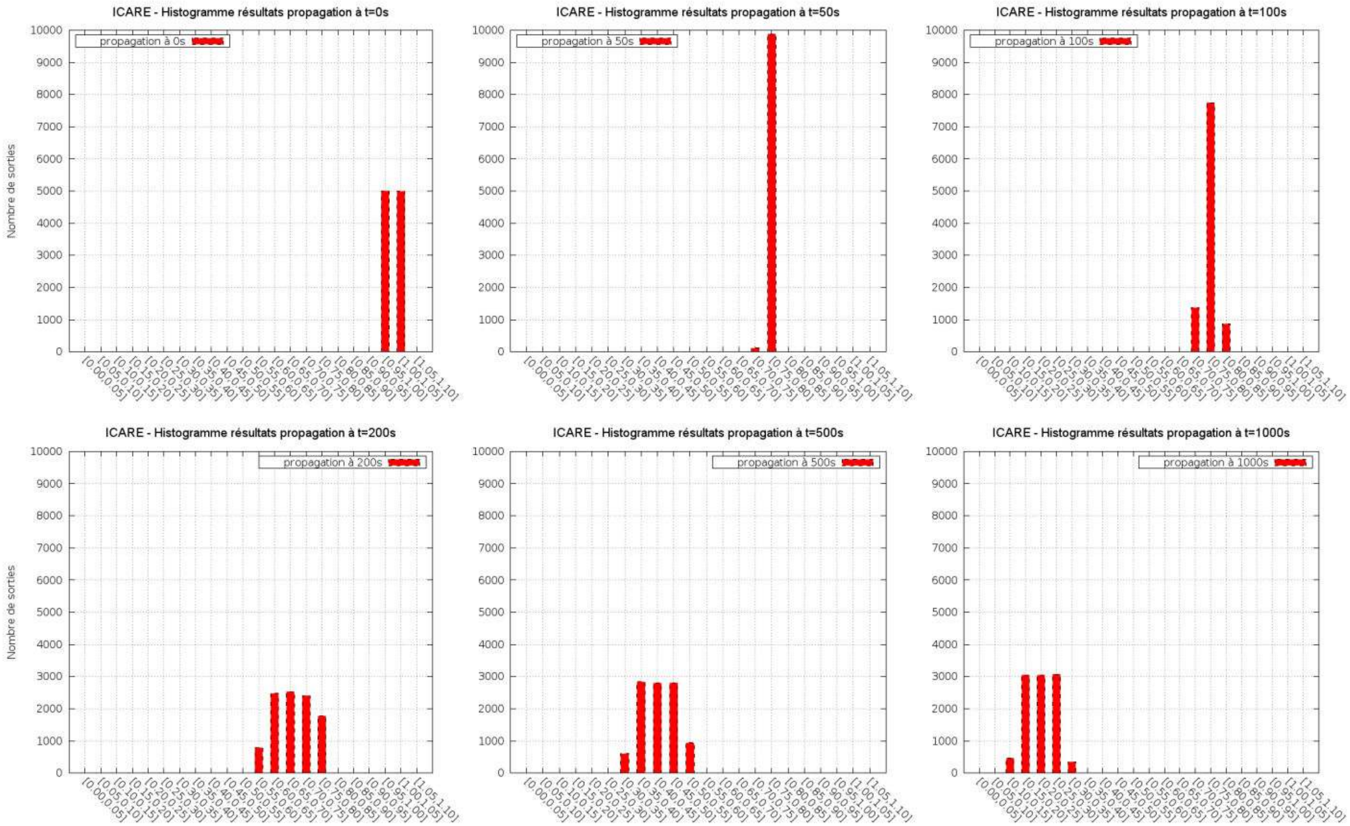


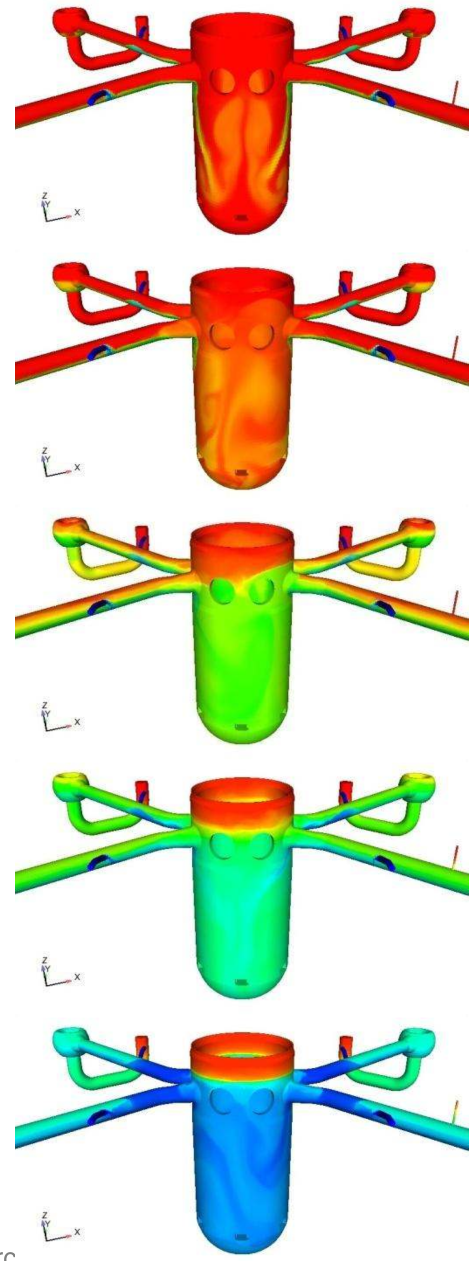


Results in an actual R&D nuclear study

- Variance due to variability of input parameters gives following results:

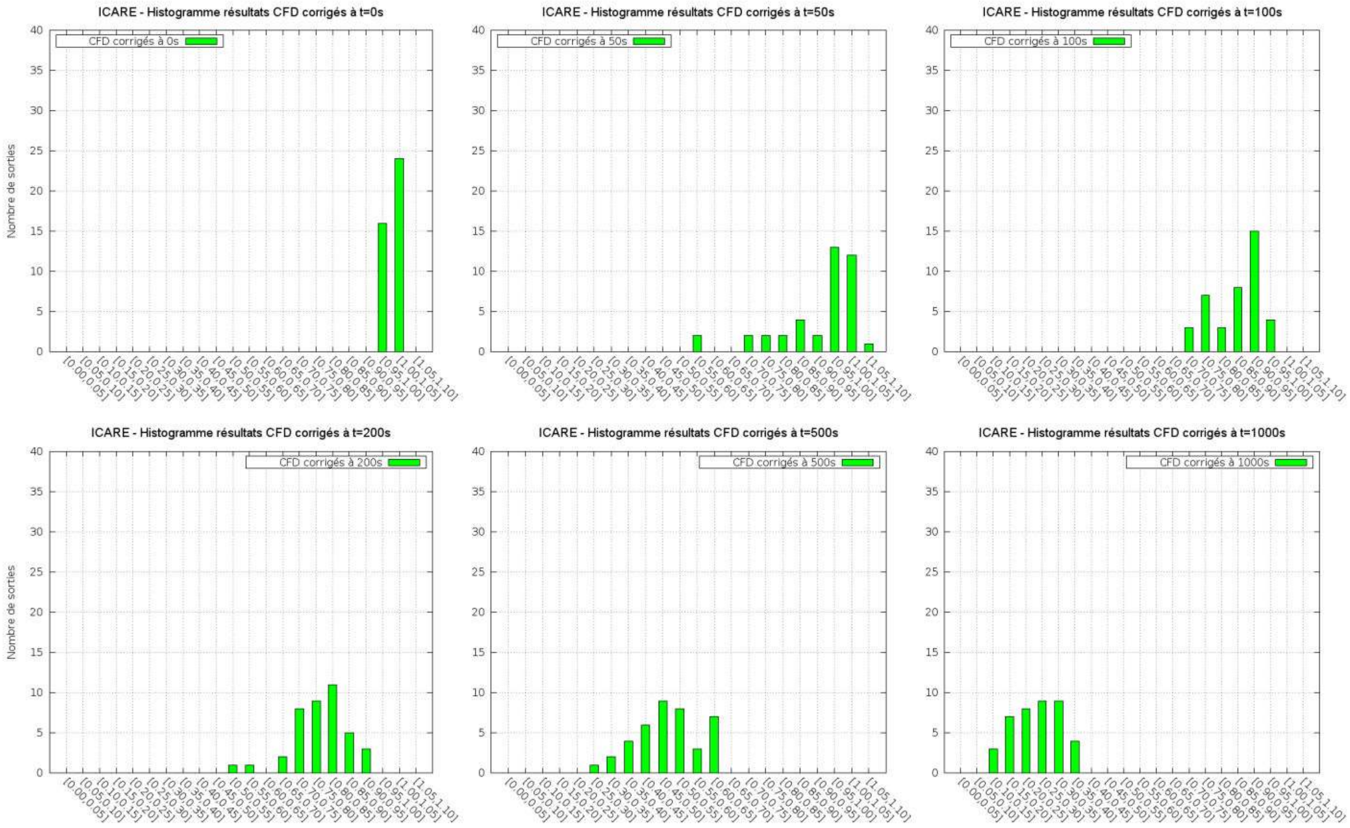
$$\mu^{C}_{PWR}(\underline{x}^{C}_{PWR}) = \sum_{i=1}^{n^{C}_{PWR}} a_i x_i + a_0$$

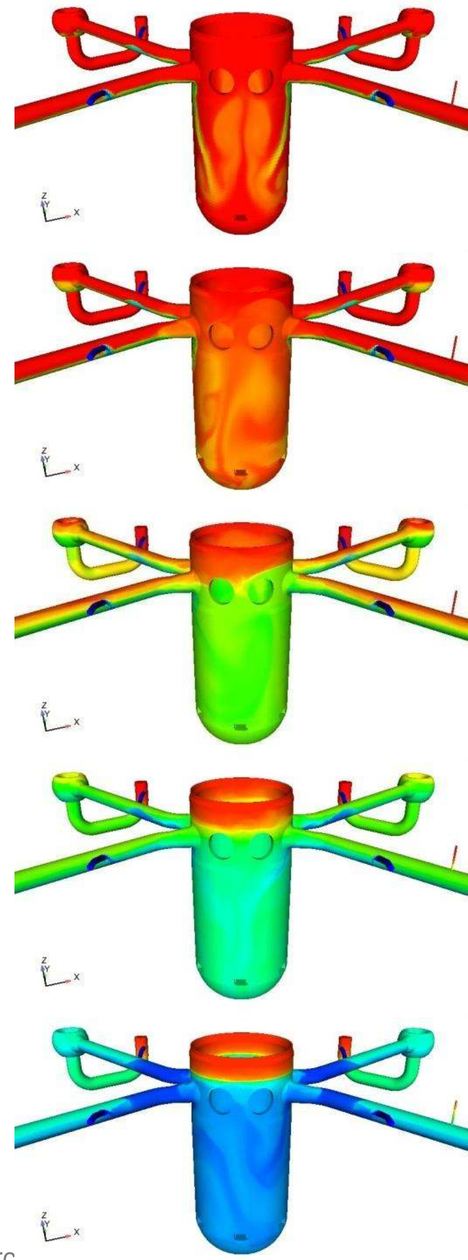




Results in an actual R&D nuclear study

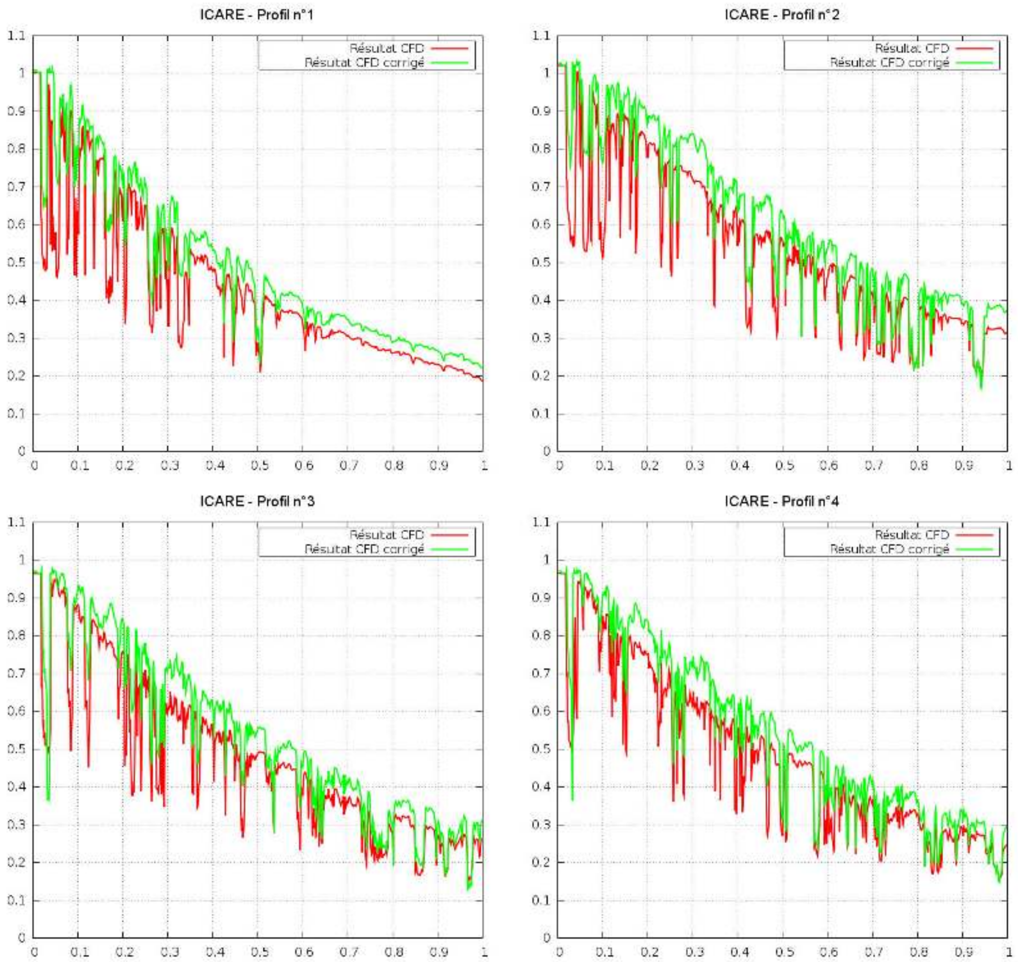
- Finally, corrected 40 CFD PWR results (note densities very different from Gaussian law):

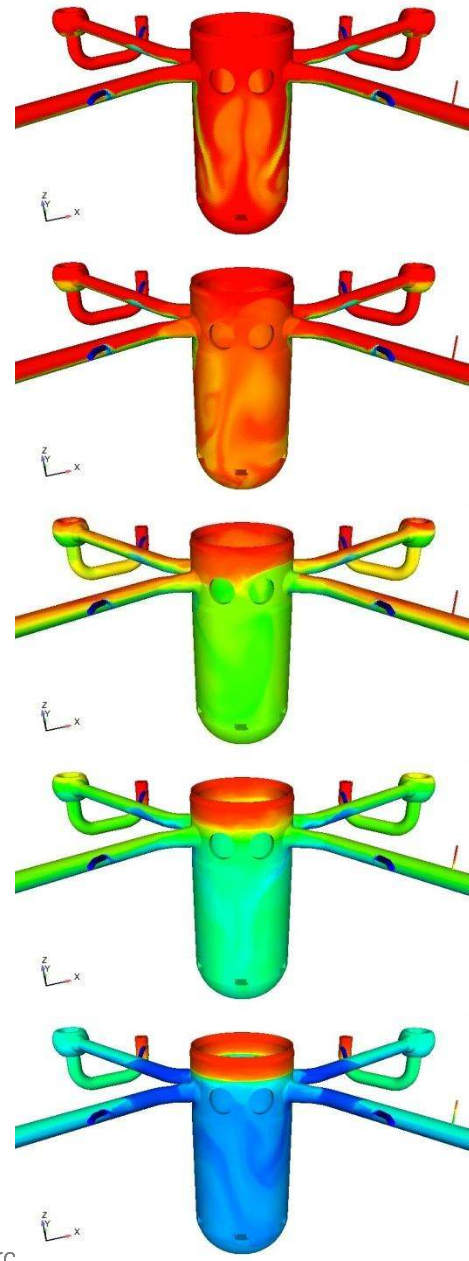




Results in an actual R&D nuclear study

- Individual (4 out of 40) corrected CFD PWR results:





Conclusions & short term prospects

- Conclusions:
  - Reasonably simple approach to deal with complex simulations.
  - Available in a verified code.
  - Recent development: estimate of uncertainties due to limited size of datasets (by bootstrap method).

- Short term prospects:
  - Use of OpenTURNS to deal with complex input uncertainties.
  - Application to other studies in nuclear domain (interest for boron dilution, hydrogen risk, …).

Thank you