Uncertainty Quantification

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SNETP Forum
TS 8 - Digitalisation - Modelling and Simulatio

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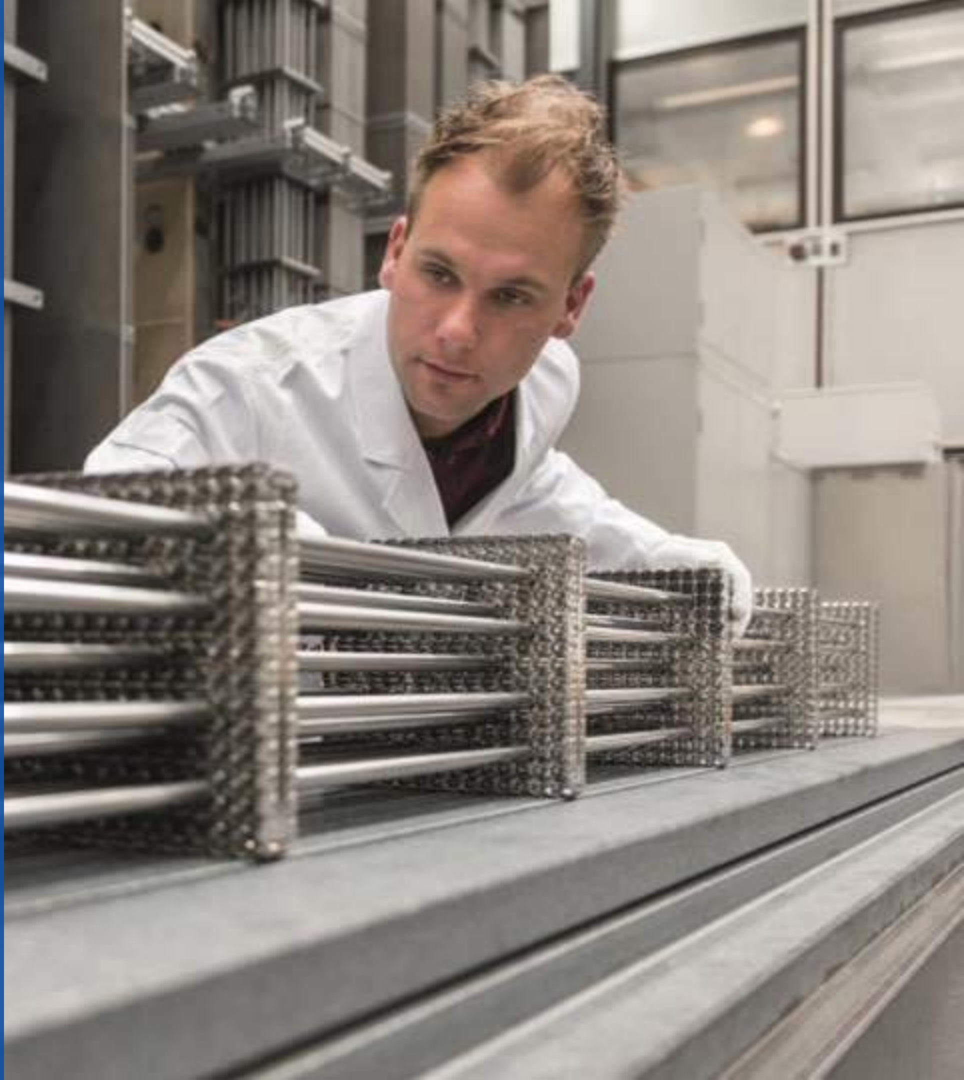


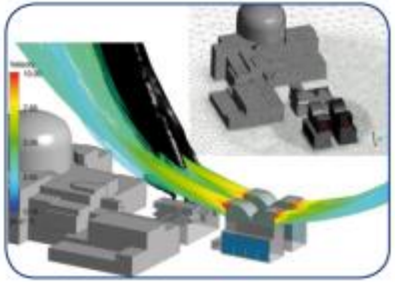
CFD @ Framatome

Framatome has a high level of competence using commercial CFD codes for more than 15 years in different codes: STAR-CCM+®, FLUENT®, OpenFOAM®, CODE SATURNE & NEPTUNE_CFD

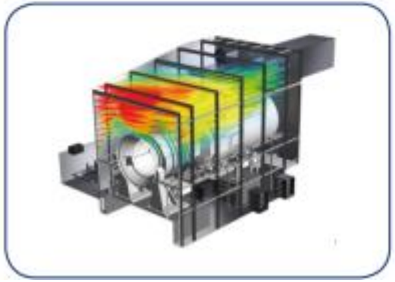
Our state-of-the-art expertise is the result of long-term experience and successful partnerships with diverse industrial organizations and research institutes

CFD analysis in the area of flow mechanics is used in applications include complex phenomena such as turbulence, multi-phase flow, chemical reactions and fluid-structure interactions:

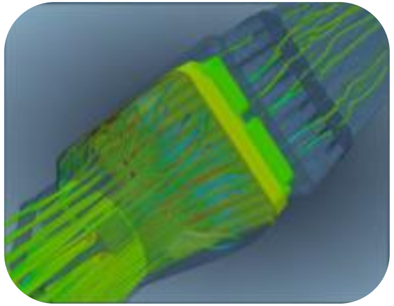
- Improving and verifying design and performance of industrial components; performing parameter studies for design optimization, lifetime extension and cost reduction in hardware
- Understanding key hydrodynamic parameters & Accomplishing root cause analysis
- Enhancing realistic load determination
- Verifying safety regulatory compliance
- Exploring innovative solutions by supporting design of experiments.



Atmospheric dispersion



Distribution of fuel gas in a gas turbine enclosure



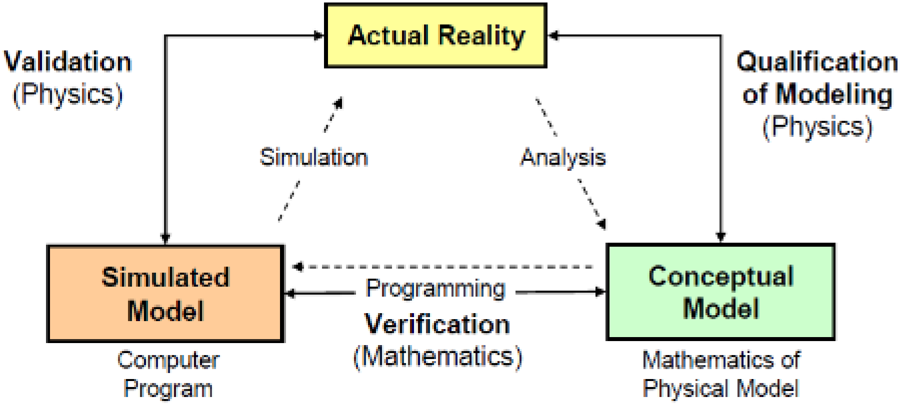
CFD Analysis of 3rd generation FUELGUARD

Modeling, Simulation and Roles of Validation & Verification

Credibility is obtained by demonstrating acceptable levels of uncertainty and error. A discussion of the uncertainties and errors in CFD simulations is provided on the page entitled Uncertainty and Error in CFD Simulations. The levels of uncertainties and errors are determined through verification assessment and validation assessment.

Verification assessment determines if the programming and computational implementation of the conceptual model is correct. It examines the mathematics in the models through comparison to exact analytical results. Verification assessment examines for computer programming errors.

Validation assessment determines if the computational simulation agrees with physical reality. It examines the science in the models through comparison to experimental results.



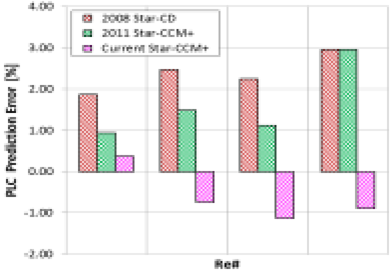
Source: NPARC Alliance CFD Verification and Validation Web Site:
http://www.grc.nasa.gov/WWW/wind/valid/homepage.html

Examples of CFD Validation @ Framatome – Spacer grid PLC Validation

Type A: Vaned Spacer Grid

AREVA's 1-Ph CFD Methods for Fuel Analysis & Design – NURETH-16 – Mathieu Martin

Type C: Helical Spacer Grid



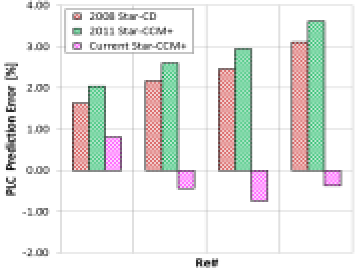
Very heterogeneous database, different design, loop, grid sizes…

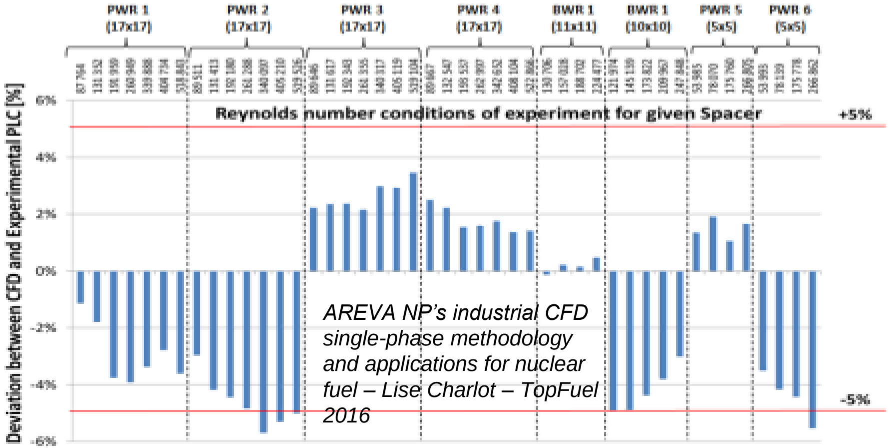
Same trend within a grid design "Family" (σ_{avg}= ± 1%)

Standard deviation on all Reynolds and tested designs is σ= ± 3%

All predictions within ± 5% of experimental values

Type B: Spacer Grid without Vanes





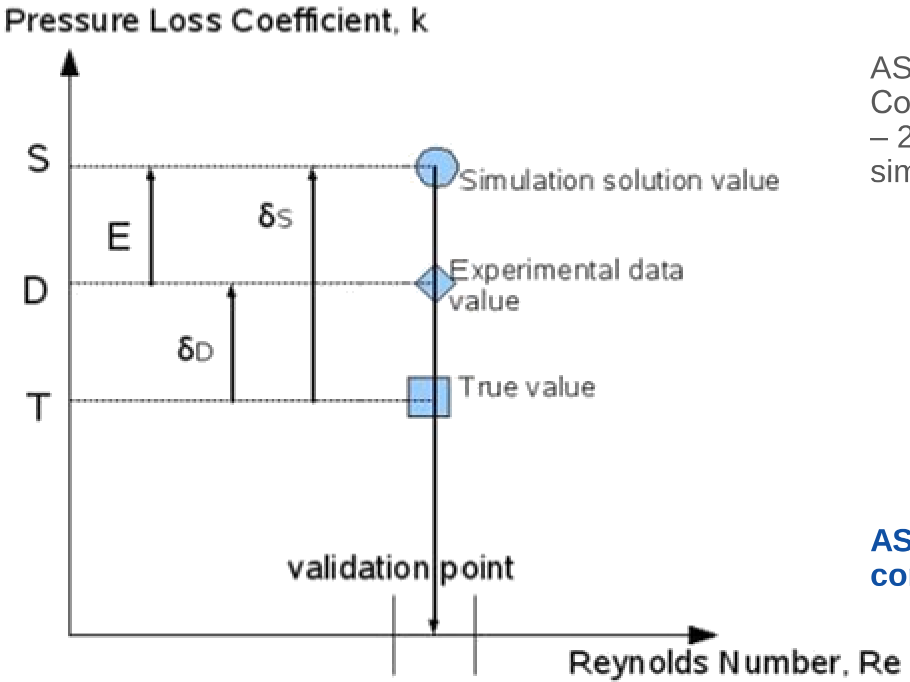
AREVA NP's industrial CFD single-phase methodology and applications for nuclear fuel – Lise Charlot – TopFuel 2016

Validation comparison error within measurement uncertainty

UQ applied to CFD – Overview of main existing methods

- PIRT (Phenomena Identification Ranking Table): efficient tool to better assess the problem's physical significant parameters
    - understand potential sensitivities; narrow down list of sources of uncertainty to only most significant input parameters
- Monte-Carlo type methods
    - high number of code runs for statistical consistency x number of input parameters = approach not viable for industrial CFD applications with today's computer capacities
- Meta-model elaboration - Polynomial Chaos Expansion (PCE)
    - some commercial softwares like ANSYS-FLUENT provide a dedicated tool; number of CFD calculations can be significant (up to a few dozens as an order of magnitude).
- Deterministic sampling
    - method which propagates uncertainty from the first statistical moments of input parameters PDFs instead of directly from PDFs, as the PDFs of the input parameters are often not known or just assumed, whereas mean values, or standard deviations can be known. Via the appropriate choice of statepoints and ponderation, it is possible to achieve uncertainty propagation with a limited number of calculations
- ASME VVUQ method
    - ties together experimental comparison and uncertainty evaluation, evaluating separately input parameter contribution to global combined validation uncertainty.
    - evaluation of the model uncertainty, provided that the experimental error is known.

Overview of ASME V&V20



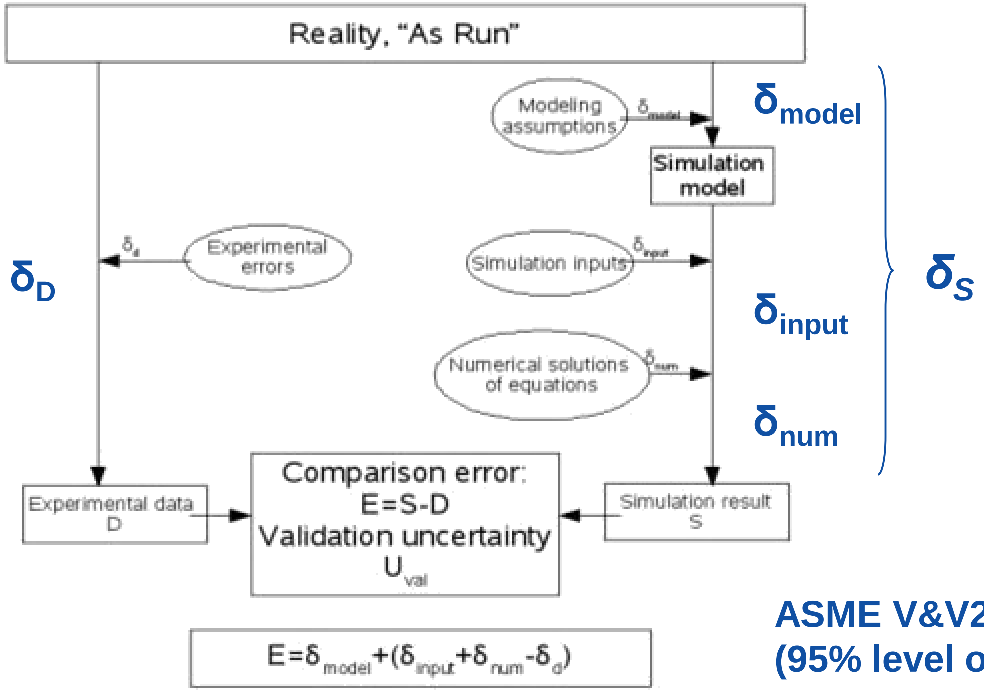
NURETH, May 12th – 17th, 2013 in Pisa - Application of the ASME V&V20 to predict Uncertainties in CFD Calculations - C. Lascar

ASME V&V20: “Standard for Verification and Validation in Computational Fluid Dynamics and Heat Transfer” V&V 20 – 2009 – revised in 2010 based on comparison of CFD simulated value to experimental value

- Objective: evaluate the uncertainty due to the modeling, δ_S
- δ_D is known from Framatome’s large amount of PLC experiments
- E = validation comparison error is known from Framatome PLC validation between CFD & experiment

ASME V&V20 provides a method to evaluate components of δ_S

Overview of ASME V&V20 (cont'd)



$$\delta_{model} = E - \delta_{num} - \delta_{input} + \delta_d$$

$$\delta_{model} \in \left[E \pm u_{val}\right]$$

with $$u_{val} = f\left(u_{num}, u_{input}, u_d\right)$$

u_{val}: validation standard uncertainty

ASME V&V20 provides a method to determine U_{val} (95% level of confidence)

Code & Solution Verification

1- Code verification

consists of establishing the correctness of the code itself

e.g.: error evaluation for a known solution

Assumed to be performed by Code Vendor

2- Solution verification

process to estimate Unum, numerical aspect of the simulation (discretization error) & has 2 origins

U_i: iteration error (resolution of the non linear equations) <0.1% by tight convergence criteria

U_h: space discretization error (space discretization of the region where the equations are solved)

Simulations assumed to be converged: $U_i \ll U_{num}$

Both different from Validation

agreement of the simulation model results with physical data from experiments

$$U_{num} = U_h$$

Grid Convergence Index Method

Grid Convergence Index (GCI) method based on the Richardson Extrapolation :

- Assumption: the PLC solution *k* have a power series representation as a function of the grid spacing *h*

$$k_i(h_i) = k_{ext} + a h_i^p + o(h_i^p)$$

  - p = order of convergence
  - h = mesh size of the simulation
  - k_{ext} = extrapolated solution

$$h = \left(\frac{\sum_{cells} Volume}{Number\ of\ cells} \right)^{1/3}$$

- Numerical uncertainty given by:

$$U_{num} = F_s \left| \delta_{RE} \right|$$

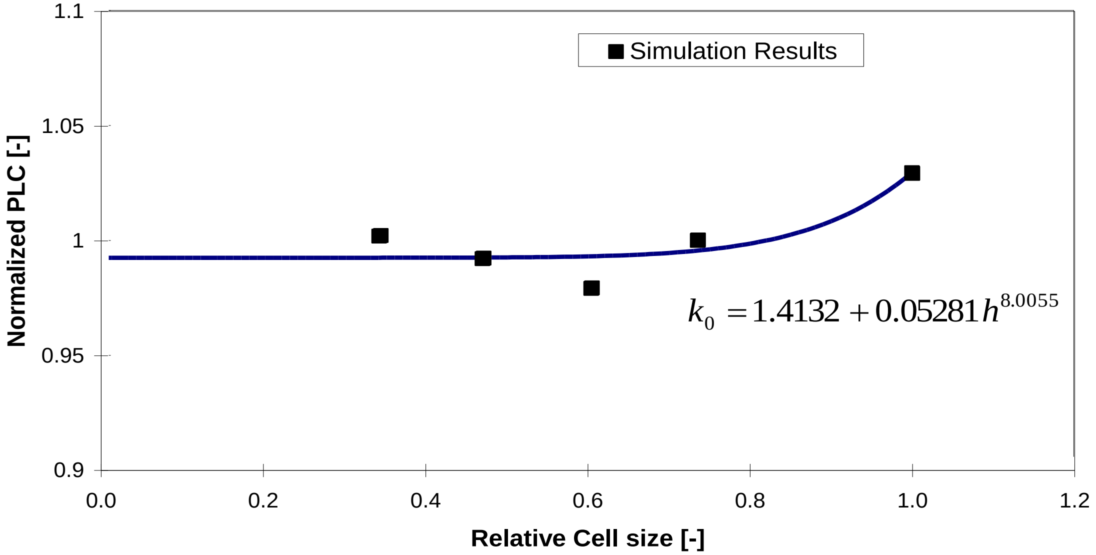
Fs: safety factor & $\delta_{RE} = a h_i^{\,p}$

- Constraints:
  - Min. 3 refined meshes are necessary to define the unknown
  - Monotonic convergence (prerequisite from the Richardson Extrapolation)
  - Refinement rate above 1.3 (Recommendation from ASME V&V20)
  - The minimum cell size must not be to small compared to the prism layer thickness

Grid Convergence Index Method – Application to CFD Simulations

CFD refined mesh solutions: No monotonic convergence

- Power series extrapolation fitted with the results : Order of convergence: p = 8.0



$$k_0 = 1.4132 + 0.05281 h^{8.0055}$$

$$R(k_0, a, p) = \sqrt{\sum_1^{n_s} \left(k_i - (k_0 + ah^p)\right)^2}$$

Oscillatory convergence common for industrial meshes

a - Application of the ASME V&V20 to predict Uncertainties in CFD Calculations - C. Lascar

Least-Squares Version of the Grid Convergence Index Method

This method within the frame of GCI has been developed by Luís Eça and Martin Hoekstra

- “Discretization Uncertainty Estimation based on a Least Squares version of the Grid Convergence Index” 2nd workshop on CFD Uncertainty Analysis, Lisbon, October 2006
- Based on the magnitude of the order of convergence

p > 2: case of a super-convergence

- $U_{num} = F_s|\delta_{RE}|$ is not reliable
- *p* should be fixed to 2, theoretical value for simple laminar flow (2^{nd} order convergence in CFD)
- In order to obtain a better *p* value by simulation, a mesh study has been performed on a simpler case: model without spacer to improve the mesh quality. In that case *p = 3.8*
- The numerical uncertainty is given by:

$$U_{num} = \max(1.25|\delta_{RE}| + U_\sigma, \quad 1.25\Delta_M)$$

$$\boxed{U_\sigma = \sqrt{\frac{\sqrt{\sum_1^{n_s}\left(k_i - (k_0 + ah^p)\right)^2}}{n_s - 3}}}$$

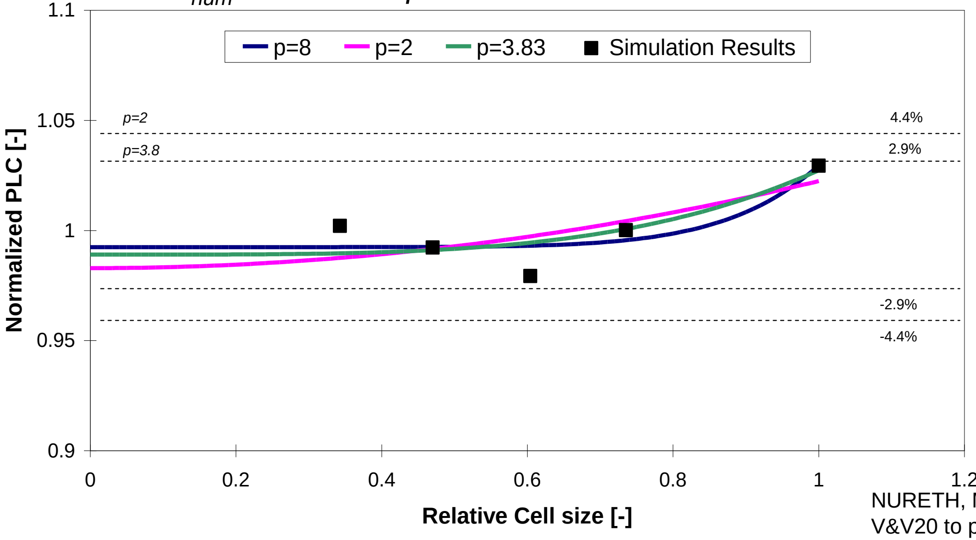
$$\boxed{\Delta_M = \max_{1\le i,j\le n_s}\left(|k_i - k_j|\right)}$$

$$\boxed{\delta_{RE} = ah^p}$$

Least-Squares Version of the GCI Method – Application to CFD Simulations

Least-Squares version of the GCI Method from Luís Eça and Martin Hoekstra successfully applied

- U_{num} = 4.4 % for p = 2
- U_{num} = 2.9 % for p = 3.8



The resulting numerical uncertainty for the typical mesh setup: ~4.4% of the pressure loss

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Uncertainty due to the Input Parameters

Input parameters

- Physical & model input parameters in CFD
  - e.g.: Roughness - E and Kappa are kept constant (inner part of a model)
- Impact of the CAD geometry

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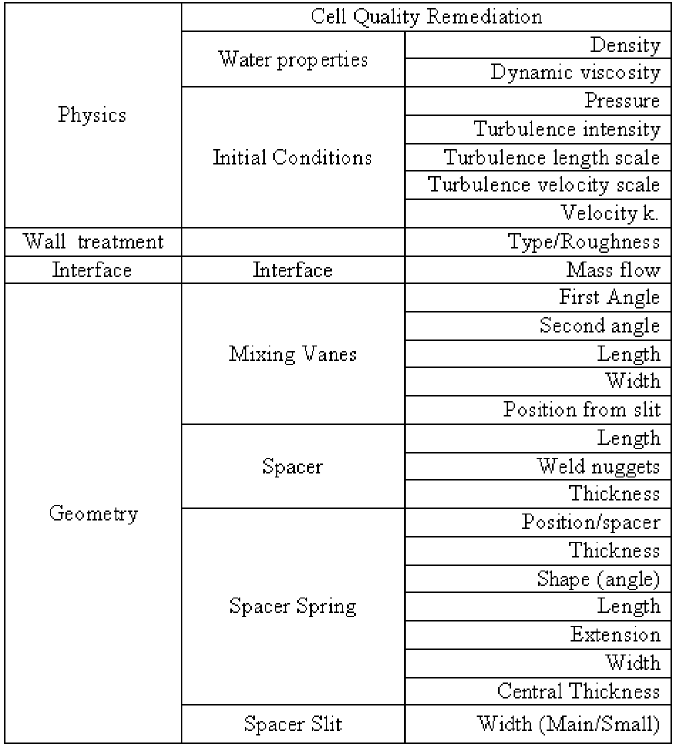


Physics	Cell Quality Remediation	
	Water properties	Density
		Dynamic viscosity
	Initial Conditions	Pressure
		Turbulence intensity
		Turbulence length scale
		Turbulence velocity scale
		Velocity k.
Wall treatment		Type/Roughness
Interface	Interface	Mass flow
Geometry	Mixing Vanes	First Angle
		Second angle
		Length
		Width
		Position from slit
	Spacer	Length
		Weld nuggets
		Thickness
	Spacer Spring	Position/spacer
		Thickness
		Shape (angle)
		Length
		Extension
		Width
		Central Thickness
	Spacer Slit	Width (Main/Small)

Presentation of Sensitivity Coefficient Method

Objective: calculate the sensitivity of the solution to each input

- Method used: "**Sensitivity Coefficient Method**"
  - Response of the system in a small (local) neighborhood of the nominal parameter vector
- Sensitivity, coupled with the standard uncertainty of the input gives U_{input}
  - if the n considered input parameters are uncorrelated

$$U_{input}^2 = \sum_i^n \left(\overline{X}_i \frac{\partial k}{\partial X_i} \frac{U_{X_i}}{\overline{X}_i} \right)^2$$

How to calculate each sensitivity coefficient?

$$\frac{\partial k}{\partial X_i} = \frac{k(X + \Delta X_i) - k(X - \Delta X_i)}{2\left\| \Delta X_i \right\|}$$

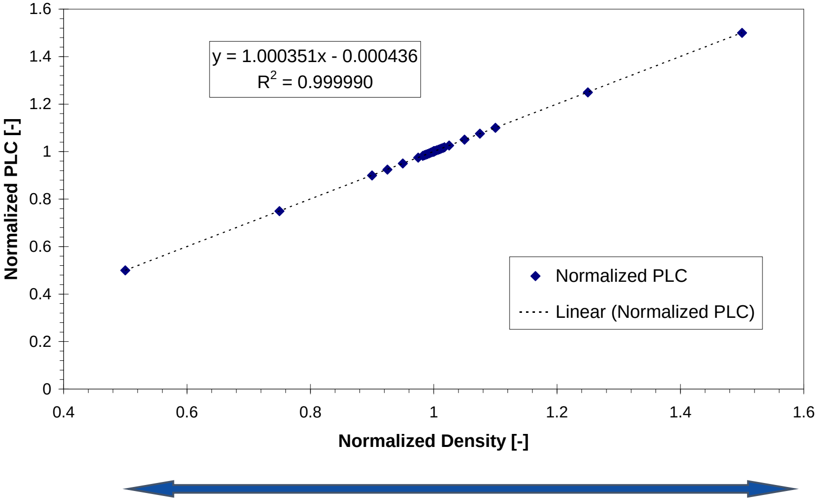
- How to choose ΔX_i ?

How to calculate U_{X_i} ?

Sensitivity Coefficient – How to determine ΔX_i ?

Determination of Sensitivity as a function of input

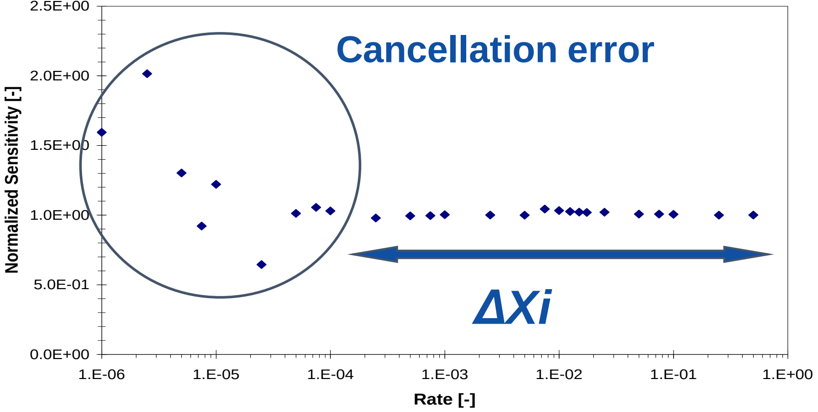
- Instead of only 2 points to calculate the sensitivity, a linear regression is done for each parameter



Which range to determine sensitivity?

Different values for ΔX_i have to be tested

- Sensitivity coefficient can be calculated for different ΔX_i



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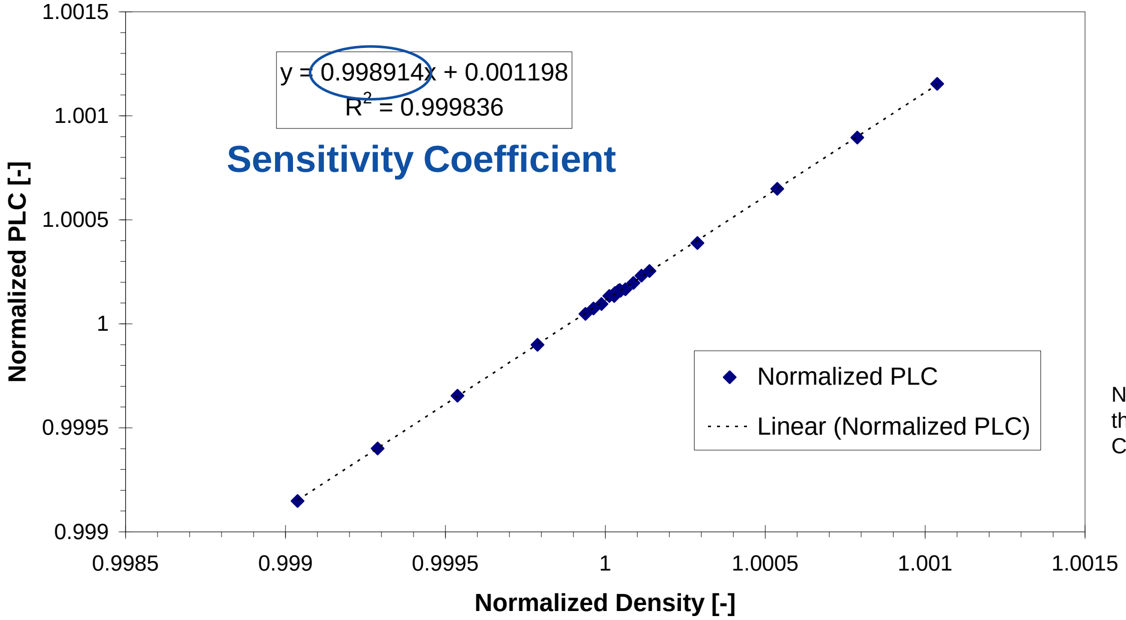
Sensitivity Coefficient – Final Value

Determination of Sensitivity as a function of input

- a linear regression is done



$y = 0.998914x + 0.001198$

$R^2 = 0.999836$

Sensitivity Coefficient

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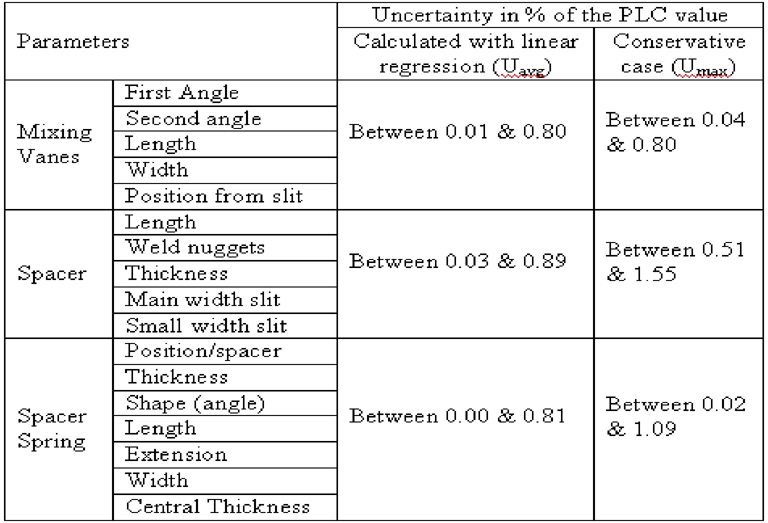
Sensitivity Coefficient – Overview

Geometric Parameters

- Physical effect of a slightly change in geometry is not linear
- Influence from discretization error
  - Remeshing is needed

2 uncertainties calculated

- Linear regression U_{avg}
- Bounds defined by the maximal acceptable geometrical deviations
  - U_{max} defined as the largest sensitivity possible with the four values



Parameters		Uncertainty in % of the PLC value	
		Calculated with linear regression (U_{avg})	Conservative case (U_{max})
Mixing Vanes	First Angle	Between 0.01 & 0.80	Between 0.04 & 0.80
	Second angle		
	Length		
	Width		
	Position from slit		
Spacer	Length	Between 0.03 & 0.89	Between 0.51 & 1.55
	Weld nuggets		
	Thickness		
	Main width slit		
	Small width slit		
Spacer Spring	Position/spacer	Between 0.00 & 0.81	Between 0.02 & 1.09
	Thickness		
	Shape (angle)		
	Length		
	Extension		
	Width		
	Central Thickness		

The input parameters uncertainty covers in total a wide range of parameters

- ***9 physical parameters & 17 geometrical parameters***

Validation Standard Uncertainty – Outcome

First-of-kind calculation of uncertainties related to a CFD calculation for nuclear fuel application in the open literature with the ASME V&V20 method

Validation Standard Uncertainty Uval for CFD PLC calculations in rod bundles

  - Uval between 4.8% (averaged case & p = 3.8) & 6.1% (conservative case & p = 2) of the pressure loss

CFD modeling to predict pressure losses in rod bundle is optimal

- E < Uval : E is lower than the upper limit of the possible error due to the CFD modeling assumptions and approximations
- Modeling error within the "noise level" imposed by the numerical, input, and experimental uncertainties
- Improving the CFD modeling is not possible without an improvement on the numerical, geometric and experimental errors

Framatome CFD modeling Best Practices for predicting pressure losses (in general 1-phase and 2-phase) in rod bundle are optimal regarding uncertainties imposed by the experiments and the code

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Thank you for your attention!