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# On the trustworthiness of simulation-based uncertainty evaluations for industrial measurement instruments like CMMs

ENBIS Spring meeting *"Trustworthy Industrial Data Science"*

Dortmund, 15 May 2024

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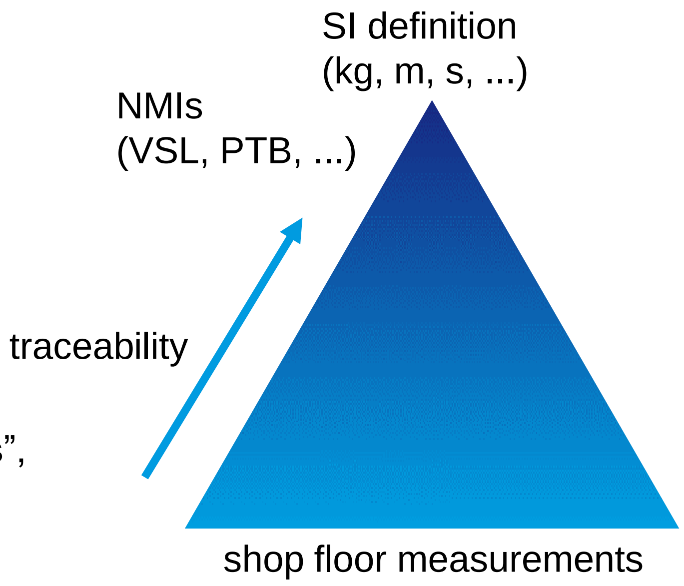
# Background

- Metrology is the science of measurement

- VSL is the National Metrology Institute (NMI) of the Netherlands, maintaining the highest measurement standards

- Cooperation within Europe:
  - Euramet
  - European Metrology Network (EMN) Mathmet
  - EPM research projects, e.g., 22DIT01 ViDiT, "Trustworthy virtual experiments and digital twins", www.vidit.ptb.de

- EMN Mathmet cooperates with ENBIS:
  - joint members
  - joint workshops, special sessions at conferences
  - ENBIS is member of the EMN Mathmet 'Stakeholder Advisory Committee'
  - ENBIS Measurement Uncertainty Special Interest Group (MU SIG) is very close to EMN Mathmet

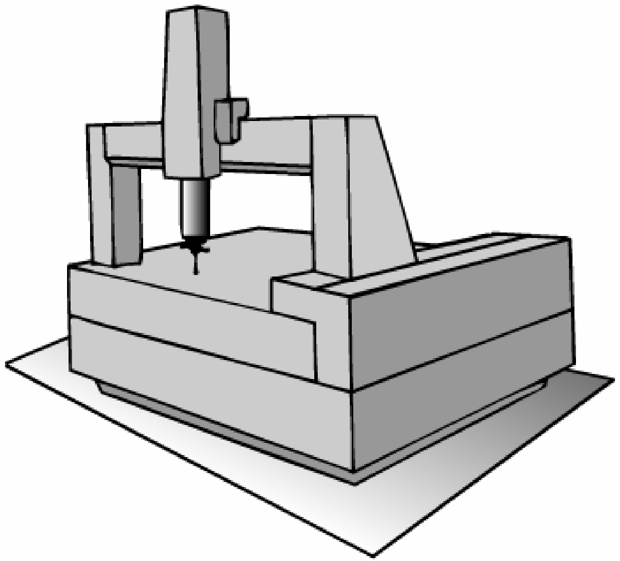


# Virtual Experiments in metrology

- A software-based simulation tool: $X = g(Y, Z)$ or $X = g_0(Y, Z) + \epsilon$ or ...
  - $Y$... measurand (quantity to be determined)
  - $X$... measured data, often involving repeated measurements
  - $Z$... other uncertain parameters, often unknown but fixed value (though fully random is not excluded)
  - $\epsilon$... random measurement noise (if not included in $g$)

- It helps:
  - understanding the measurement process
  - analyzing the effect of error sources
  - optimizing the measurement scheme
  - optimizing the data analysis after the measurement

- Examples:
  - Coordinate Measurement Machines
  - Tilted Wave Interferometry, Scatterometry
  - Flow (CFD) & flow meter simulations



Lehrstuhl Qualitätsmanagement und Fertigungsmesstechnik, Prof. A. Weckenmann https://commons.wikimedia.org/wiki/File:Koordinatenmesssystem_in_Portalbauweise_(Animation).gif 

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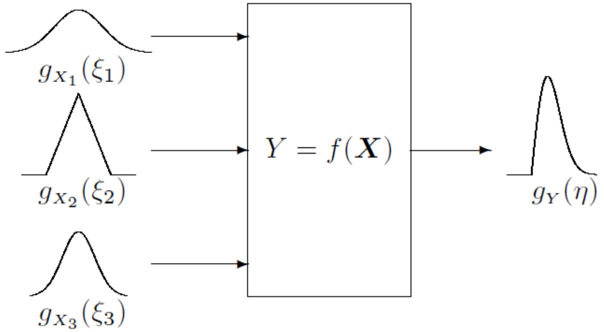
# Uncertainty evaluation in metrology

$$u_c^2(y) = \sum_{i=1}^{N} \left( \frac{\partial f}{\partial x_i} \right)^2 u^2(x_i)$$

- GUM suite of documents:
  - Guide to the evaluation of Uncertainty in Measurement (JCGM-100): propagation of variances ('LPU')
  - Additional documents: propagation of distributions, multivariate case, modelling, conformity assessment

- Main focus on measurement model: $Y = f(X, Z)$
  - $Y$... measurand (quantity to be determined)
  - $X$... measured data, often involving repeated measurements
  - $Z$... other uncertain parameters, often unknown but fixed value




- Propagation of distributions (using a Monte Carlo method) is often seen as 'gold standard'

- Evaluation of long-run success-rates (LSRs) in the context of a statistical model is not so common

- When a VE is available, it is a small step to evaluate the LSR of a data analysis method (DA)

- We assessed LSRs for several GUM-inspired DAs

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# Scenario: Simplified Coordinate Measuring Machine (CMM)

**Data *X*:**

- $(x_i, y_i)$ coordinates of 25 to 1000 measured points on a circle

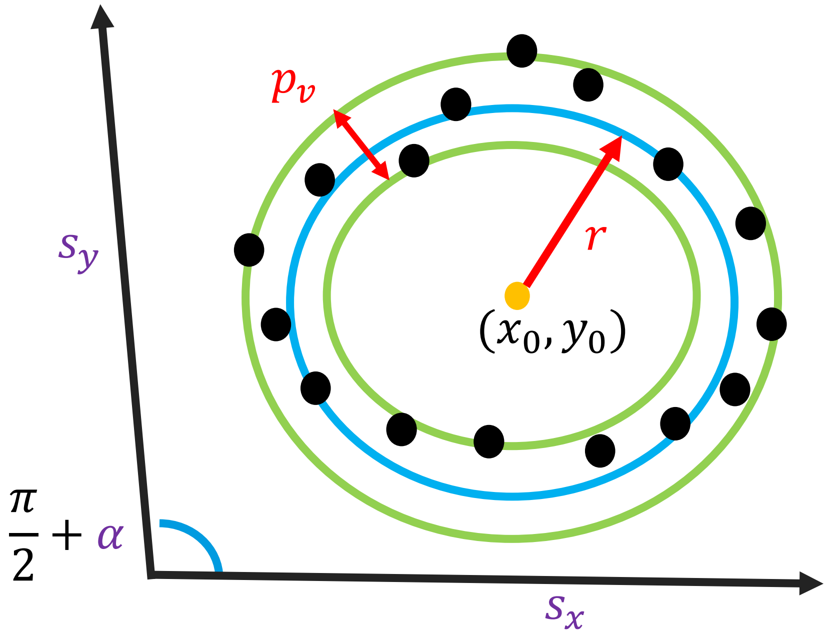
**Measurand and artefact related parameters *Y*:**

- Measurand:
  - Circle radius $r$
  - Roundness PV-value $p_v$
- Auxiliary parameters:
  - Circle centre $(x_0, y_0)$
  - Probing directions $\varphi_i$
  - Lobe parameters: $n_{\text{lob}}$, $\varphi_{\text{lob}}$, $a$ $(= p_v/2)$

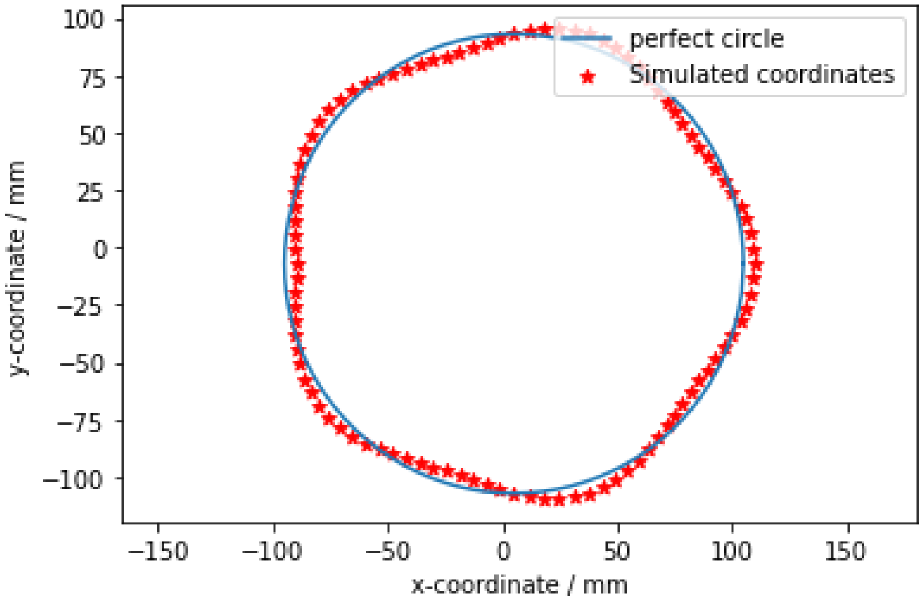
**Parameters *Z*:**

- Instrument parameters:
  - Scale errors of x- and y-axis: $s_x$, $s_y$
  - Squareness deviation between x- and y-axis: $\alpha$
  - Std. dev. of measurement noise $\sigma$
- Data analysis parameters:
  - Gaussian filter cut-off parameter $f_{\text{cut}}$

- $X = g(Y, Z) + \epsilon$
- $\varphi_i = 2\pi i/n$
- $r_i = r + \sin(\varphi_{\text{lob}} + \varphi_i\, n_{\text{lob}})$
- $x_{\text{true},i} = x_0 + r_i \cos(\varphi_i)$
- $y_{\text{true},i} = y_0 + r_i \sin(\varphi_i)$
- $\begin{pmatrix} x \\ y \end{pmatrix}_{\text{meas},i} = A \begin{pmatrix} x \\ y \end{pmatrix}_{\text{true},i} + \begin{pmatrix} \epsilon_x \\ \epsilon_y \end{pmatrix}_i$



# Classical data analysis method




- Goal: estimate $r$ and $p_v$ and their uncertainties,
  e.g., their standard deviations or 95%-coverage intervals

- Define measurement model $Y = f(X, Z)$. Here:
  1. Correct the data $X$ for any systematic errors
  2. Filter the corrected data
  3. Fit a circle to the corrected data
  4. Derive $r$ and $p_v$ from the fit results, return $Y = (r, p_v)$

- Uncertainty evaluation:
  - Data $X$ have normal distribution $\mathrm{N}(X, V_X)$, with covariance matrix $V_X$
  - Parameters $Z$ have a specified distribution with covariance matrix $V_Z$
  - Propagate variances through model $f$: $V_Y = \left(\frac{\partial f}{\partial X}\right)^2 V_X + \left(\frac{\partial f}{\partial Z}\right)^2 V_Z$ (LPU)
  - Propagate distributions through model $f$: Monte Carlo method applied to $Y = f(X, Z)$ (PoD)

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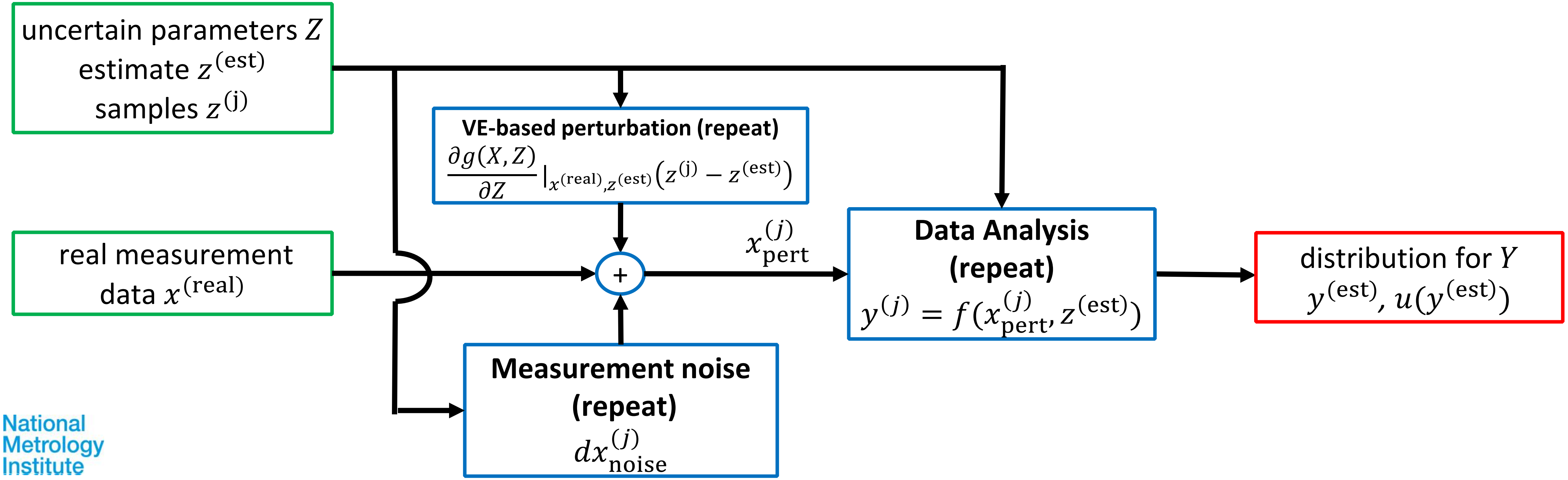
# VE-based perturbation analysis

- Idea:
  - Analyze how the data $X$ would change if the unknown, fixed value of $Z$ changes.
  - Evaluate the perturbed data, yielding a range of `reasonable values' for the measurand $Y$

- $P(Y) = PoD_{P(dX_{\mathrm{noise}}),P(Z)}\left(f\left(x^{(\mathrm{real})} + \frac{\partial g(X,Z)}{\partial Z}|_{x^{(\mathrm{real})},z^{(\mathrm{est})}}\left(Z - z^{(\mathrm{est})}\right) + dX_{\mathrm{noise}}, z^{(\mathrm{est})}\right)\right)$

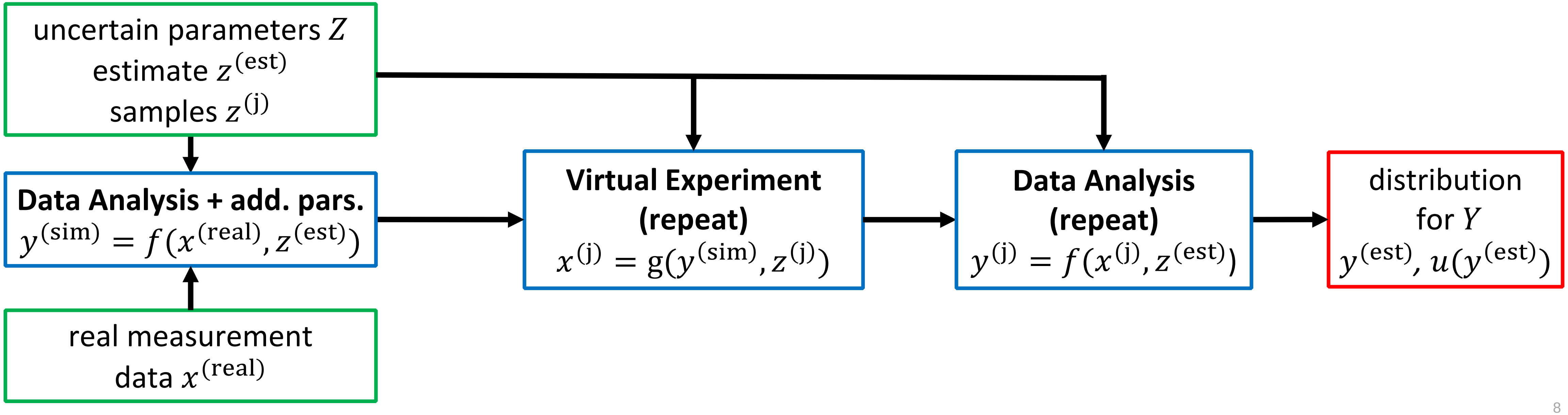


# VE-based uncertainty prediction

- Idea: A VE can be used to analyze a measurement and predict an uncertainty. (PoD-via-VE)

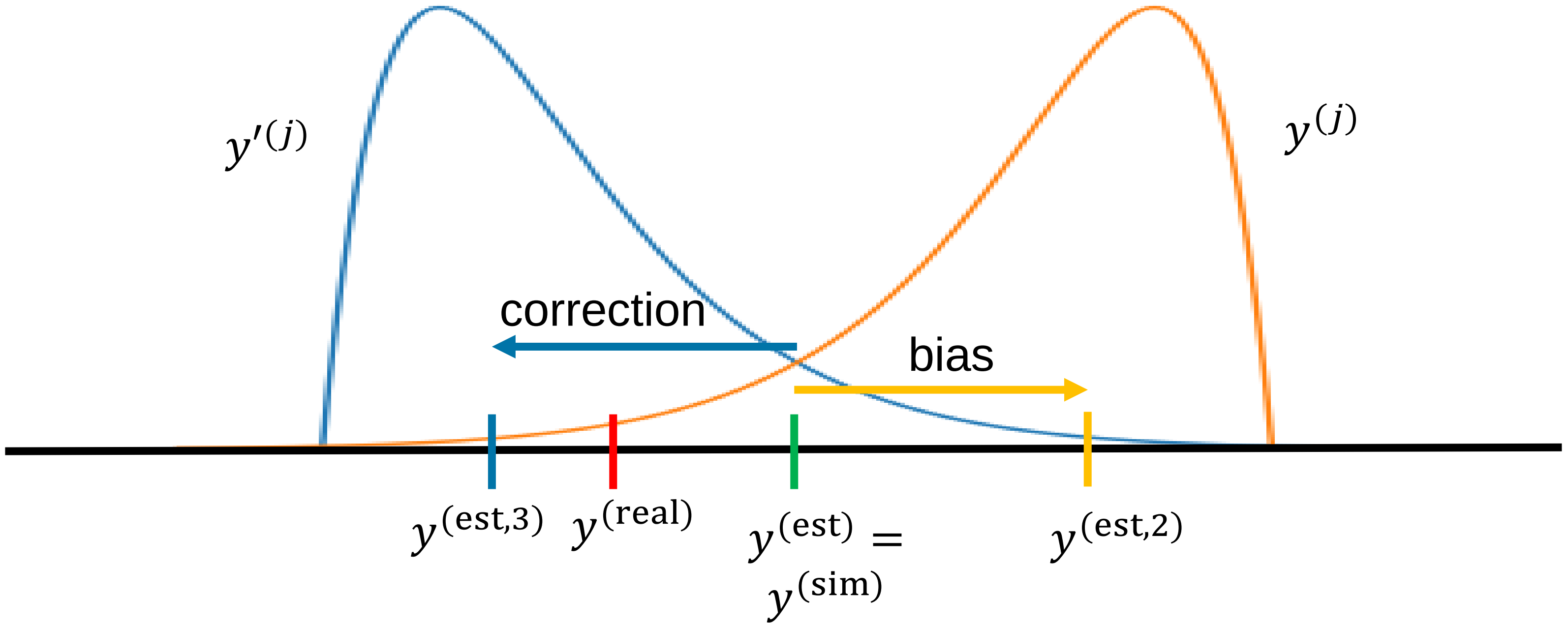
Steps:

1. Determine an $y^{(\mathrm{sim})}$ to be used in the VE by evaluating $f(x^{(\mathrm{real})}, z^{(\mathrm{est})})$ and additional parameter estimates
2. Repeatedly run the VE using different samples $z^{(j)}$ of $Z$ and the noise $\partial x_{\mathrm{noise}}^{(j)}$ related to $X$, resulting in $x^{(j)}$
3. Evaluate for each run $y^{(j)} = f\left(x^{(j)}, z^{(j)}\right)$
4. Compute the quantities of interest from the $y^{(j)}$, e.g., mean, standard deviation, 95%-coverage intervals



# Bias-corrected VE-based analysis

- Problem: If the model is strongly non-linear, the result of $f(X,Z)$ can be biased, i.e., $E(f(X,Z)) \neq y^{\text{true}}$
- Solution idea: Add a bias correction to the generated samples $y^{(j)}$ based on VE experiments
- Resulting corrected samples: $y'^{(j)} = 2y^{(\text{sim})} - y^{(j)}$

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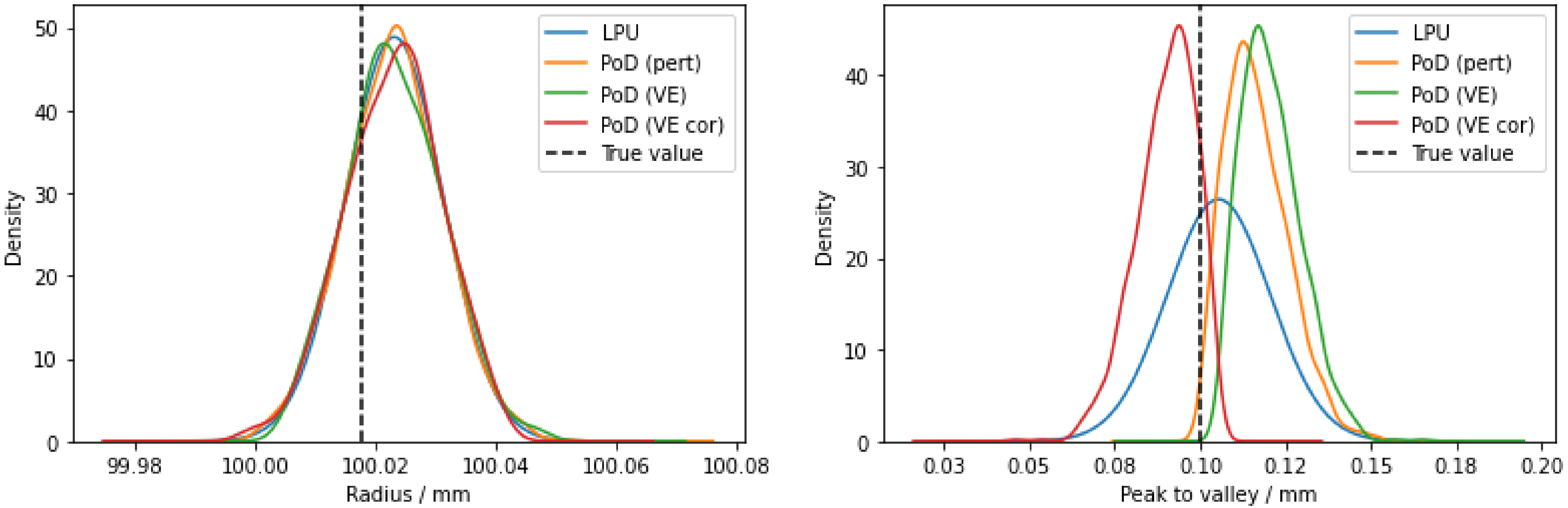
# Results - distributions

- For a relatively **smooth measurand** like the radius, all methods give very **similar results**
- For a **non-linear measurand** like the roundness PV-value, the results are **quite different**

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# Results – Uncertainties & Long-run success rates

- For radius all methods return proper estimates
- PV-value is overestimated by PoD (pert) and PoD (VE) resulting in 0 LSR
- Uncertainties are quite different

| Uncertainty method | average of the $\hat{r} \pm U(\hat{r})$ / mm | average of the $\hat{p}_v \pm U(\hat{p}_v)$ / mm |
|---|---|---|
| True value | 100.018 | 0.100 |
| LPU | 100.018 $\pm$ 0.016 | 0.115 $\pm$ 0.027 |
| PoD (pert) | 100.018 $\pm$ 0.016 | 0.125 $\pm$ 0.021 |
| PoD (VE) | 100.018 $\pm$ 0.016 | 0.134 $\pm$ 0.017 |
| PoD (VE cor) | 100.018 $\pm$ 0.016 | 0.096 $\pm$ 0.017 |

(Average of 1000 runs)

| Uncertainty method | LSR radius | LSR PV-value |
|---|---|---|
| Target value | 95 % | 95 % |
| LPU | 96 % | 90 % |
| PoD (pert) | 95 % | 0 % |
| PoD (VE) | 95 % | 0 % |
| PoD (VE cor) | 95 % | 95 % |

# Robustness w.r.t. VE artefact shape for $\hat{p}_v$ results

- Calculated uncertainties are not sensitive to exact shape used inside the VE
- LPU does not use an assumed shape
- PoD (pert) only depend on derivative of VE, which is in this case quite insensitive to artefact shape
- Estimating PV-value without modelling it does not work for PoD (VE) and PoD (VE cor)

| VE artefact model | 5-lobed circle | 10-lobed circle | perfect circle |
|---|---|---|---|
| True value | 0.100 | 0.100 | 0.100 |
| LPU | 0.115±0.027 | 0.115±0.027 | 0.115±0.027 |
| PoD (pert) | 0.125±0.021 | 0.125±0.021 | 0.125±0.021 |
| PoD (VE) | 0.134±0.017 | 0.132±0.017 | 0.022±0.018 |
| PoD (VE cor) | 0.096±0.017 | 0.098±0.017 | 0.209±0.018 |

(Average of 1000 runs)

| VE artefact model | 5-lobed circle | 10-lobed circle | perfect circle |
|---|---|---|---|
| Target value | 95 % | 95 % | 95 % |
| LPU | 90 % | 90 % | 90 % |
| PoD (pert) | 0 % | 0 % | 0 % |
| PoD (VE) | 0 % | 0 % | 0 % |
| PoD (VE cor) | 95 % | 96 % | 0 % |

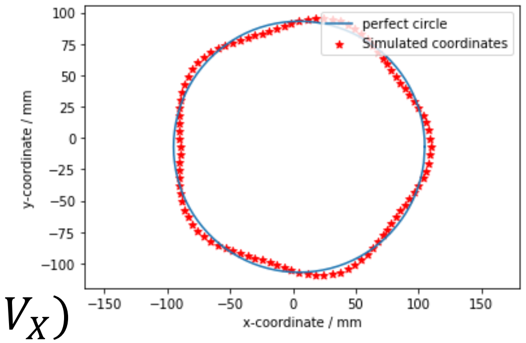
# Conclusions

- Virtual Experiments in metrology enable a thorough assessment of data analysis methods used in industrial measurements

- Trustworthiness of some uncertainty evaluation methods is questionable in the light of long-run success rates calculated with the help of VEs for highly non-linear measurands

- Unbiased estimate depends on the value of the uncertainty, not only on the measured values and best estimates of the parameters. No conservative uncertainties allowed anymore!

# Appendix: Bayesian inversion




- Given priors $P_0(Y)$ and $P_0(Z)$ and likelihood $L(X;Y,Z) = P(X \mid Y,Z) \sim N(g(Y,Z),V_X)$

  calculate posterior distribution $P(Y,Z \mid X) \sim P(X \mid Y,Z)P_0(Y)P_0(Z)$

  and marginal distribution for the measurand $P(Y \mid X)$

- Challenges:
  - Linear scale errors and radius error can compensate each other, leading to unrealistic solutions
  - An accurate model of the artefact shape is needed, otherwise residuals are not correctly distributed
  - In a more complex VE, there may be many more uncertain parameters in $Z$, and the Bayesian inference problem becomes computationally prohibitely large
  - For more complex VEs involving multiple `low-level’ noise contributions, the likelihood may not have an analytical expression, making the uncertainty evaluation quite complex