Physikalisch-Technische Bundesanstalt
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National Metrology Institute

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Metrology for virtual measuring instruments

Methods of uncertainty evaluation using virtual experiments with the example of the tilted-wave interferometer

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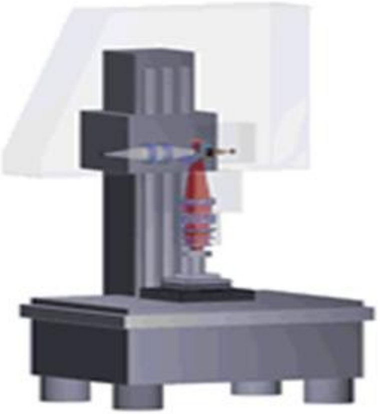
[1] *Physikalisch-Technische Bundesanstalt, 8.42 Data Analysis and Measurement Uncertainty*
[2] *Physikalisch-Technische Bundesanstalt, 4.24 Asphere Metrology*

Tilted-Wave Interferometer (TWI)

- Interferometric form measurement of optical aspheres and freeform surfaces

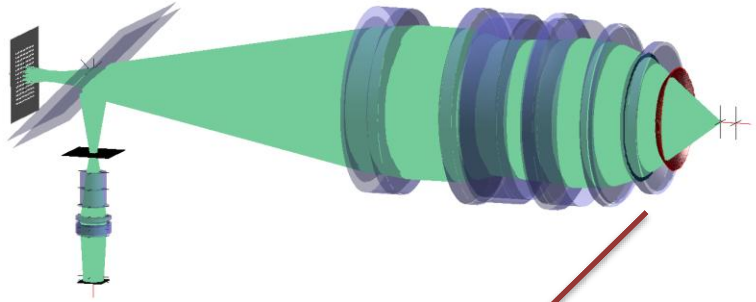
- Invented at the Institute of Applied Optics (ITO, University of Stuttgart); further developed jointly with Mahr and PTB.

- PTB has developed its own evaluation software and virtual experiment for the measurement procedure.

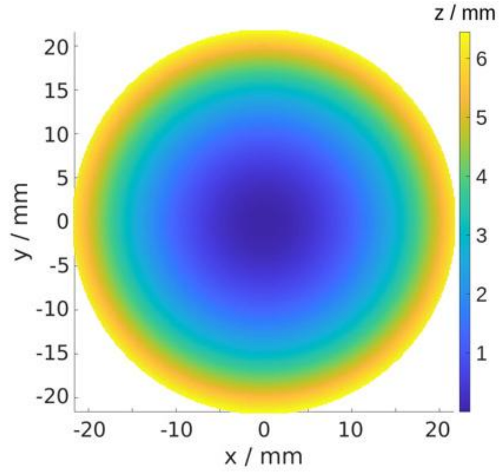


TWI reconstruction using virtual experiments (VE)

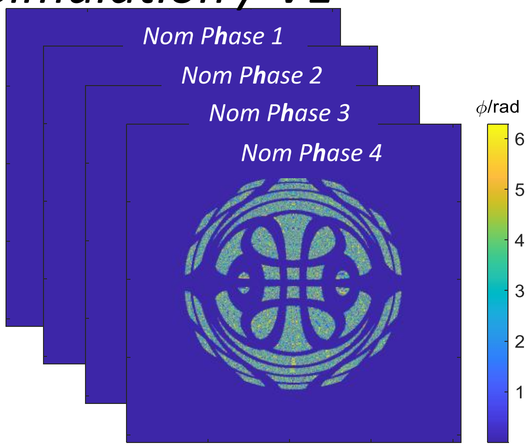
VE mimics real device



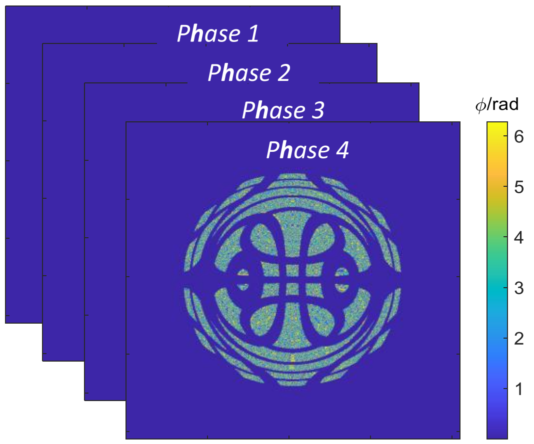
Measurand (Topography)



Simulation / VE



Observation



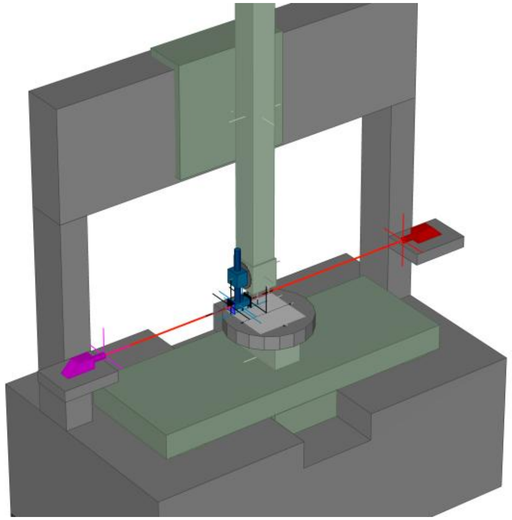
$$res = \min_{(T,pos)} \|Observation - VE(T,pos)\|$$

Inverse problem leads to measurand, i.e. topography T

SimOptDevice

PTB-inhouse developed MATLAB-Toolbox to model optical devices.

```
Machine coordinate system
|_ Tt_X
|   |_ Tt_Z
|       |_ Tr_phi
|           |_ Ts_Sensor
|               |_ Mirror_AC_X
|               |_ Sensor
|               |_ Mirror_L_I_X
|_ AC_X
|_ L_I_X
|_ Ts_down
    |_ Tt_Y
        |_ Tr_eta
            |_ Ts_Tilting_Table
                |_ Topography
```



Features

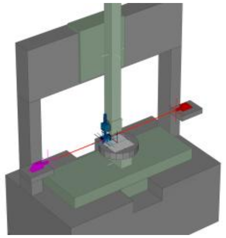
- hierarchical coordinate systems
- various geometric setups via script
- arbitrary coordinate transformation

Raytracing & Rayaiming supported

Axel Wiegmann, Manuel Stavridis, Monika Walzel, Frank Siewert, Thomas Zeschke, Michael Schulz, Clemens Elster; Accuracy evaluation for sub-aperture interferometry measurements of a synchrotron mirror using virtual experiments, Precision Engineering, Volume 3F Issue 2, April 2011, Pages 183-190, doi: https://doi.org/10.1016/j.precisioneng.2010.08.007

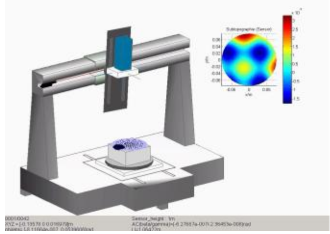
Applications (Extraction, 2005 - today)

Synchrotron Mirror



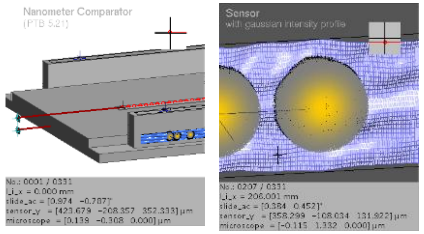
Founded Project (2005 – 2008)

Telescopic Mirror



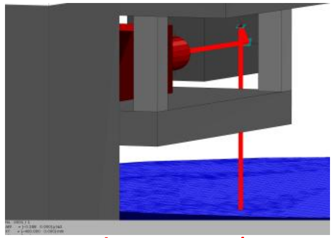
Founded Project (2012)

Nanometer Comparator



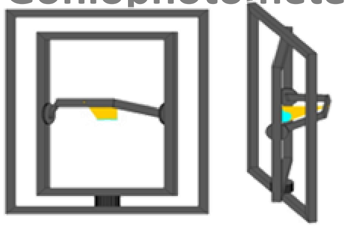
BMBF Project (2008 – 2010)

Deflectometry



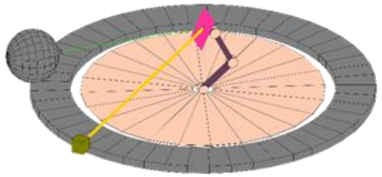
PTB internal Project (2008-2011)

Goniophotometer



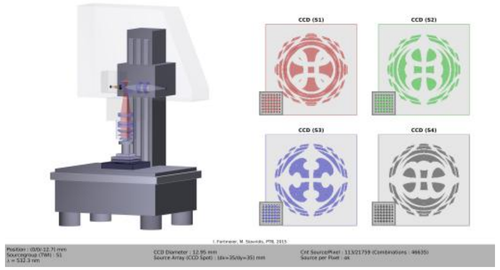
MNPQ – Project (2010-2013)
MNPQ – Project (2013-2016)

Multidimensional Reflectometry



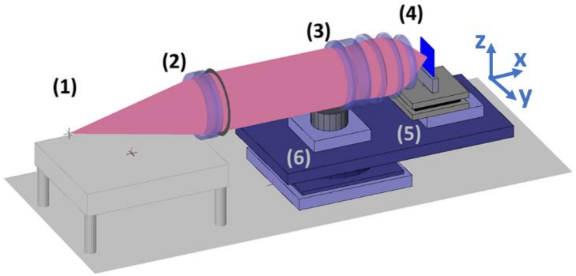
EMRP Project IND 10 (2013-2016)

Tilted-Wave Interferometer



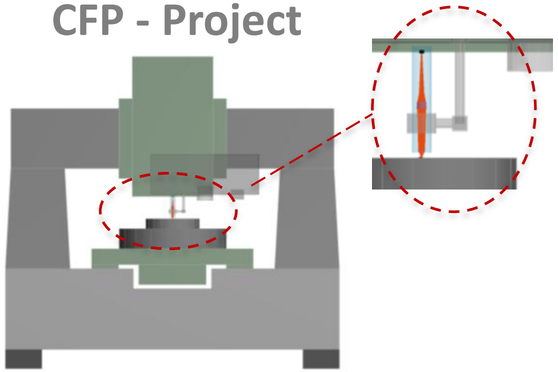
EMRP Project IND 10 (2008-2011)
EMPIR Project 15SIB01 (2016-2019)
EPM Project "ViDiT" (2023-today)

MTF – Facility



Transmet – Project (2017-2020)

CFP - Project

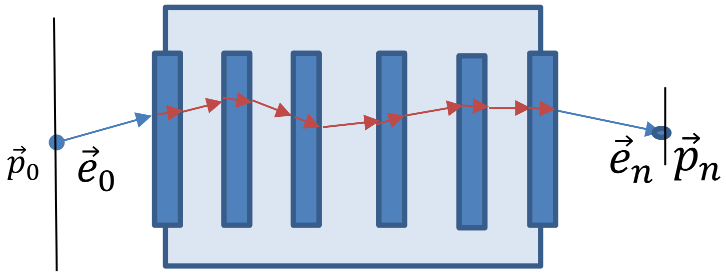


EMPIR Project "TracOptic" (2021-2024)

Modelling of Light (Ray tracing, Ray Aiming)

Ray tracing

$$[\vec{p}_n, \vec{e}_n] = f(\vec{p}_0, \vec{e}_0)$$

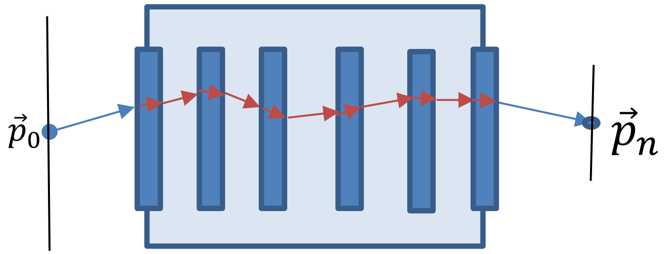


Gradient

$$\frac{\partial[\vec{p}_n, \vec{e}_n]}{\partial(\vec{p}_0, \vec{e}_0)} = f'(\vec{p}_0, \vec{e}_0)$$

Ray Aiming (nonlin. problem)

$$opl = f(\vec{p}_0, \vec{p}_n)$$ *opl: optical path length*



Gradient

$$\frac{\partial opl}{\vec{p}_i} = (n_{i-1}\vec{e}_{i-1} - n_i\vec{e}_i)$$

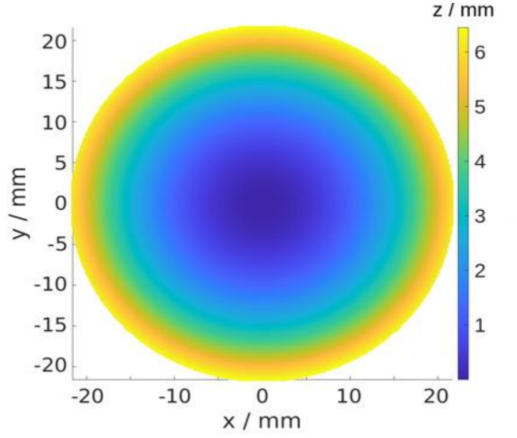
R. Schachtschneider, M. Stavridis, I. Fortmeier, M. Schulz, C. Elster, SimOptDevice: a library for virtual optical experiments, *Journal of Sensors and Sensor Systems*: 8, 105 – 110, (2019), doi: https://doi.org/10.5194/jsss-8-105-2019

I. Fortmeier, M. Stavridis, A. Wiegmann, M. Schulz, W. Osten, C. Elster, Analytical Jacobian and its application to tilted-wave interferometry, *Optics Express*: 22, 18, 13 S. (2014), doi: https://doi.org/10.1364/oe.22.021313

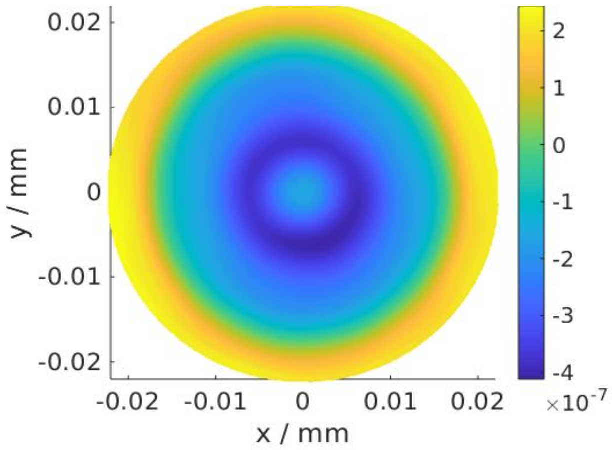
Goal: Uncertainty Evaluation

In metrology each measurement requires a measurement uncertainty.

Measurand (absolute form)



Measurand (difference form)



Uncertainty

?

Challenge:
The TWI reconstruction procedure, which involves the VE, is

- high dimensional,
- non-linear and
- computationally expensive.

Bayesian Uncertainty Evaluation (Monte Carlo)

Reference method using statistical analysis.

A suitable approximation yields a Monte Carlo sampling procedure.

$$U \approx \frac{1}{n}\sum_{i=1}^{n} \sigma^2 \left(J_{\hat{\theta},Z_i}^T J_{\hat{\theta},Z_i}\right)^{-1} + \left(\hat{\theta} - \theta(Z_i)\right)\left(\hat{\theta} - \theta(Z_i)\right)^T$$

Requires $n \gg 1000$ repetitions of the complex reconstruction procedure $\theta(Z_i)$ with different settings

Time consuming: ~16 hours to obtain the uncertainty.

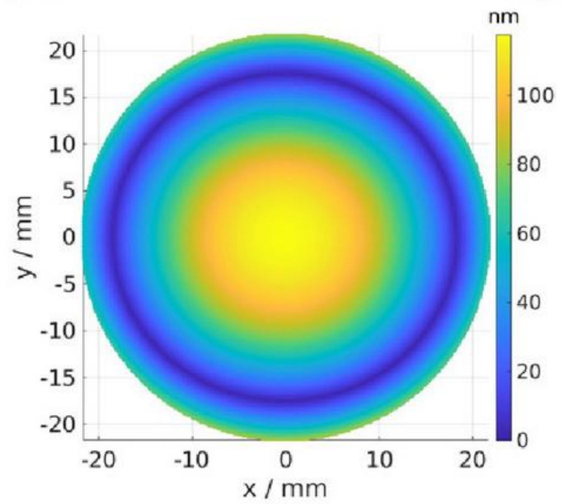
M. Marschall, I. Fortmeier, M. Stavridis, F. Hughes, C. Elster, Bayesian uncertainty evaluation applied to the tilted-wave interferometer, *Optics Express*: 32, 11, 18664 – 18683, (2024), doi: https://doi.org/10.1364/OE.524241

Application example: Toroidal surface

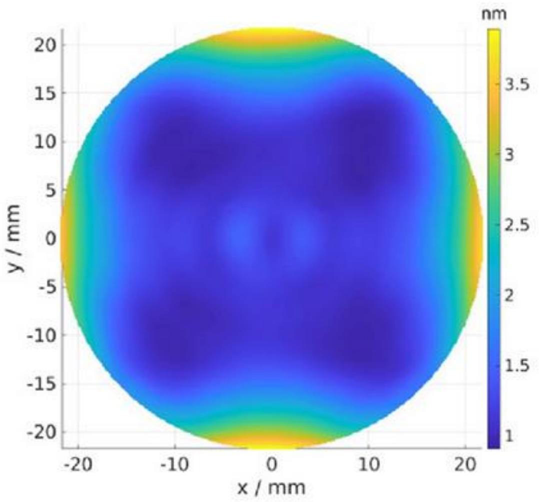
- Gaussian measurement noise with standard deviation $\sigma = 10$ nm
- Additional key influencing parameters chosen for demonstration of method:

Description of parameter	Symbol	Distribution	mean	std. uncertainty
Deviation of SUT position in x-direction	Δx	Gaussian	0 m	5×10^{-6} m
Deviation of SUT position in y-direction	Δy	Gaussian	0 m	5×10^{-6} m
Deviation of SUT position in z-direction	Δz	Gaussian	0 m	10^{-6} m
Deviation of SUT orientation in α-direction	$\Delta\alpha$	Gaussian	0 m	3×10^{-4} rad
Deviation of SUT orientation in β-direction	$\Delta\beta$	Gaussian	0 m	3×10^{-4} rad
Deviation of SUT orientation in γ-direction	$\Delta\gamma$	Gaussian	0 m	3×10^{-4} rad
Calibration parameters of wavefront manipulators	Z_{wav}	multiv. Gaussian	$\hat{Z}_{\mathrm{wav}}$	Γ_{wav}

Uncertainty



without Δz –uncertainty



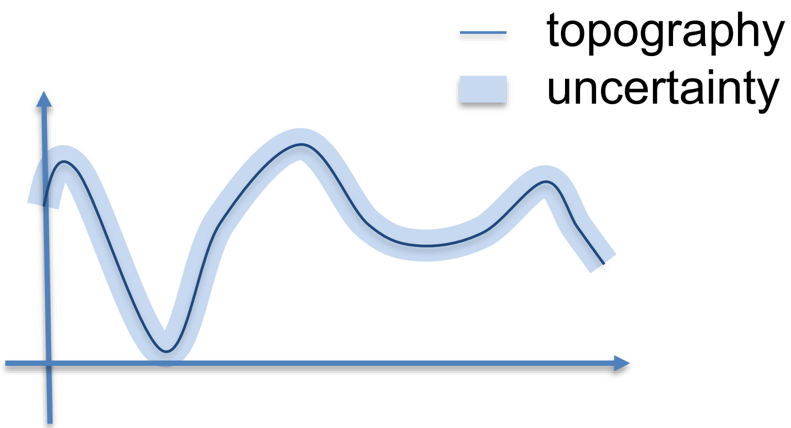
- Results show strong sensitivity with respect to certain input quanitites
- Uncertainty of input quantities is subject to current research

M. Marschall, I. Fortmeier, M. Stavridis, F. Hughes, C. Elster, Bayesian uncertainty evaluation applied to the tilted-wave interferometer, *Optics Express*: 32, 11, 18664 – 18683, (2024), doi: https://doi.org/10.1364/OE.524241

Linear Approach: Sensitivity matrices for the TWI

Approximation:

The uncertainty should be small around the actual measurand -> behaviour could be nearly linear.



Gradients can be determined analytically using SimOptDevice.

With these gradients the *law of propagation of uncertainties* is applicable.

Linearization of the measurement procedure

$y =$ measurand (topography)

$z =$ other input quantities (fixed but uncertain)

Reconstruction for measurand:

$$res = \min_{y} \| Observation - VE(y,z) \|,$$

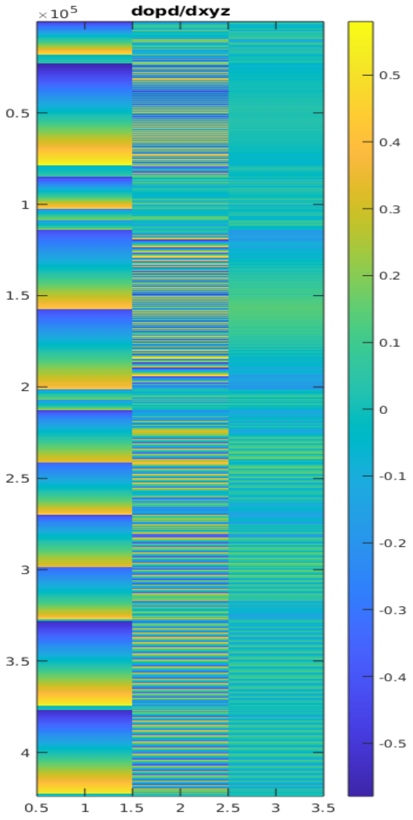
Linear Approximation:

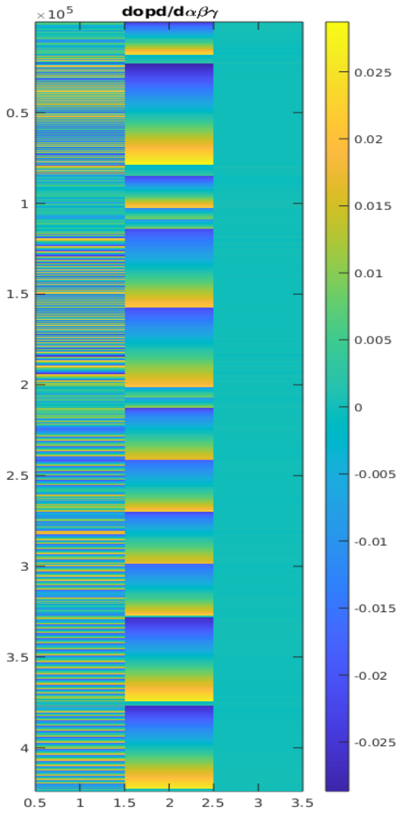
$$VE(y,z) \approx A_y y + A_z z = [A_y, A_z] \begin{bmatrix} y \\ z \end{bmatrix}$$

Solved for y:

$$y = A_y^{-1}(Observation - A_z z)$$

The linear sensitivity matrix for A_y, A_z can be analytical calculated by the TWI – Software:





Law of propagation of uncertainties (LPU)

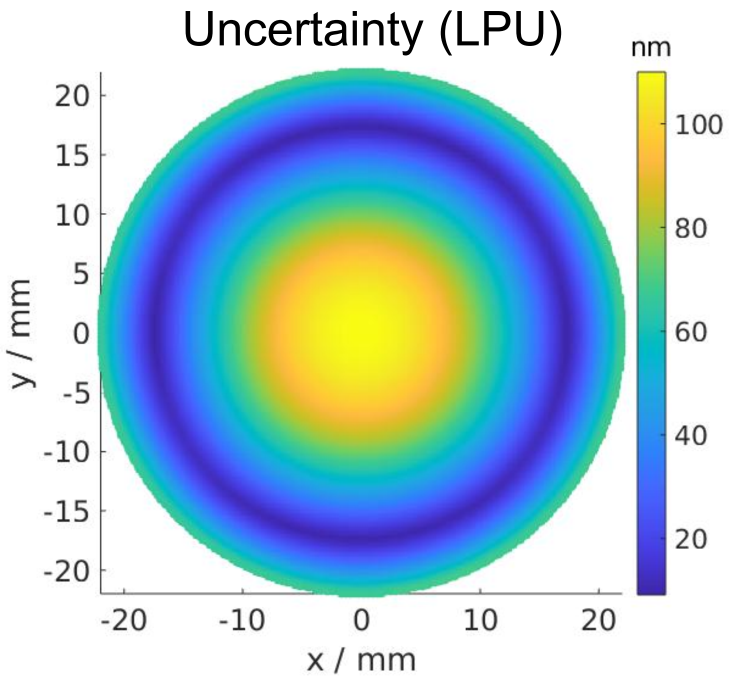
Uncertainty (covariance):

$$U = A_y^{-1}(U_x + A_z U_z A_z^T)\left(A_y^{-1}\right)^T$$

$$u = \sqrt{diag\ (U)}$$

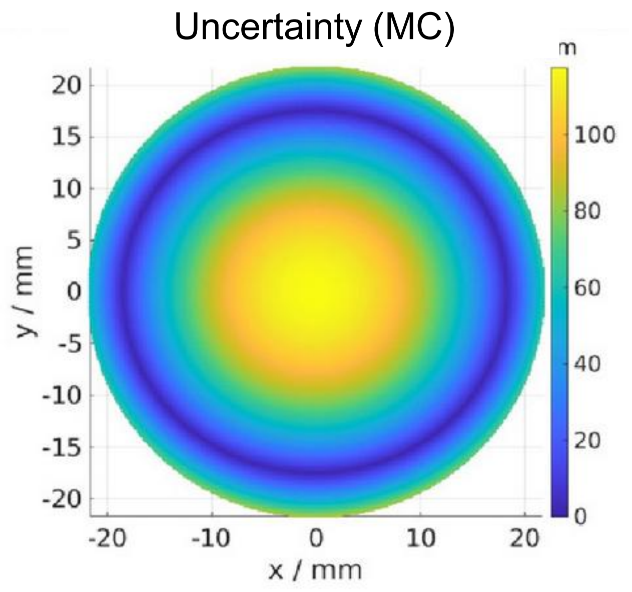
U_x = noise on measurement DOPD
U_z = uncertainty of input quantities e.g. position of specimen
A_z = linear relation measurement DOPD to u_z
A_y = linear relation measurement DOPD to measurand

computational time << 10 min

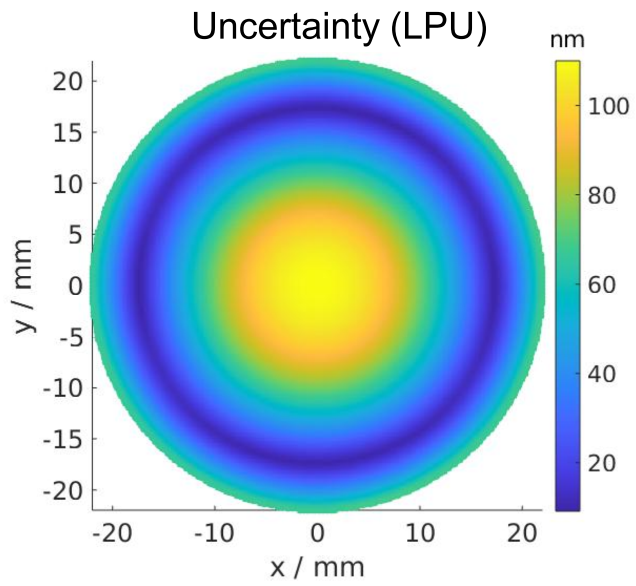


Comparison

Bayesian reference method (MC)



linear propagation of uncertainty (LPU)



Conclusion

We introduced a method to estimate the uncertainty for nonlinear virtual experiments with linear approximation.

For the TWI, this method delivers an uncertainty which is close to that of a Bayesian reference method.

It is capable of real-time uncertainty evaluation.

Outlook

- Further analysis of the linearization
- Method validation required using real world data

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