MAX-PLANCK-INSTITUT
FÜR PLASMAPHYSIK

Applications of Bayesian data analysis at W7-X stellarator

Wendelstein 7-X

Maciej Krychowiak, S. Kwak, J. Svensson, S. Bannmann, F. Henke, D. Gradic, O. Ford, R. König, et al.

EUROfusion

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- Basics of Bayesian data analysis
- Core: Core: Inference of electron density profiles and particle sources from BES
  - Complexity
- Edge: Gaussian Process Tomography of carbon radiation in divertor plasma
  - Model (hyperparameters) optimization
- Wall: Ellipsometry to measure parameters of thin layer coating on first wall components
  - Bayesian diagnostic design

Bayesian approach: constructing the posterior distribution

- Model evidence *P(D)*
  - Optimisation of model parameters (hyperparameters)

Example emission tomography

Posterior probability distribution

$$P(Z_{eff}) = \frac{P(D|Z_{eff}) \times P(Z_{eff})}{P(D)}$$

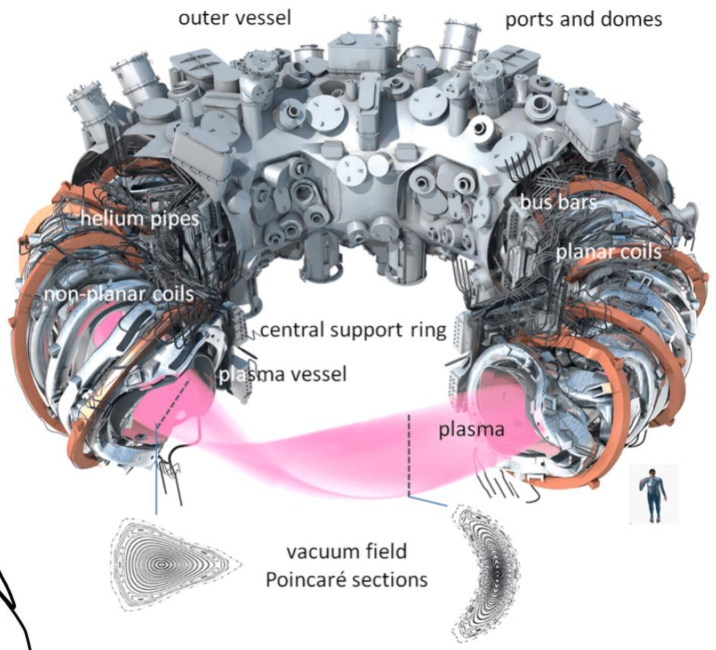
- Explore posterior distribution to find
  - ➢ Most probable solution
  - ➢ Uncertainties of inferred parameters
  - ➢ Correlations between parameters

Analysis in all three cases done in the Minerva Bayesian modeling framework

Seed eScience Research

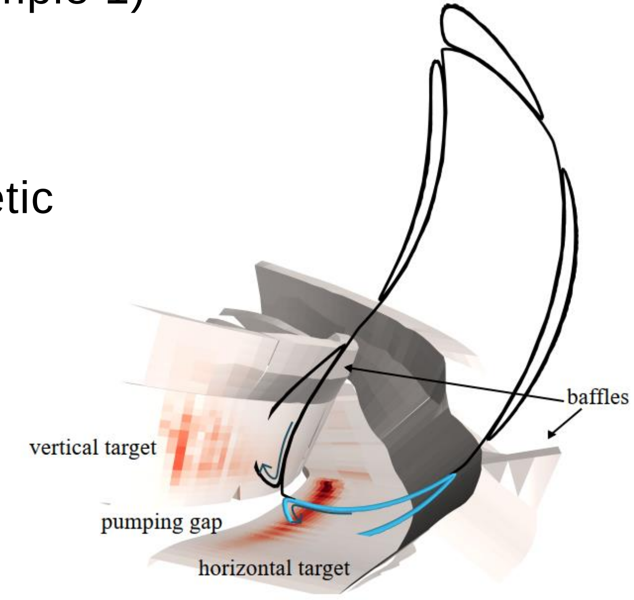
W7-X: superconducting stellarator with island divertor

- Largest stellarator in the world (R = 5 m)
- Superconducting magnetic field coils
- Long pulse operation (30 min.)
- Intensive program on plasma wall interaction (example 3)
- Optimised to reduce neoclassical transport
- Turbulent transport the major player (example 1)



Island divertor

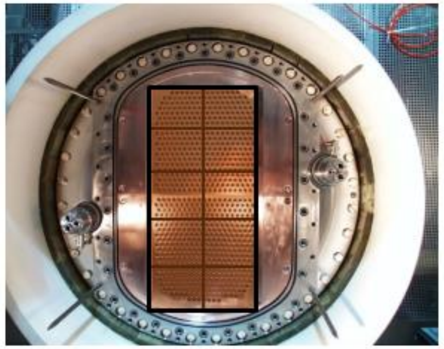
- Plasma-wall interaction defined by magnetic islands cutting divertor surface
- At 10 discrete divertor modules
- One of the goals: impurity retention
- Therefore tomographic reconstruction of impurity emission in divertor (example 2)

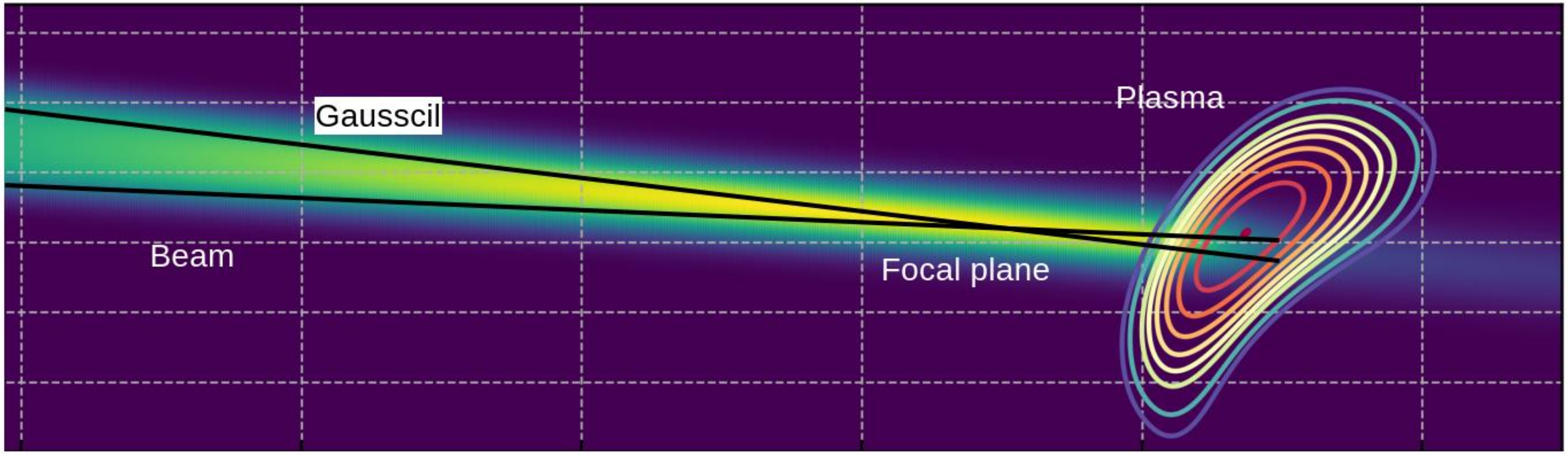


Contents

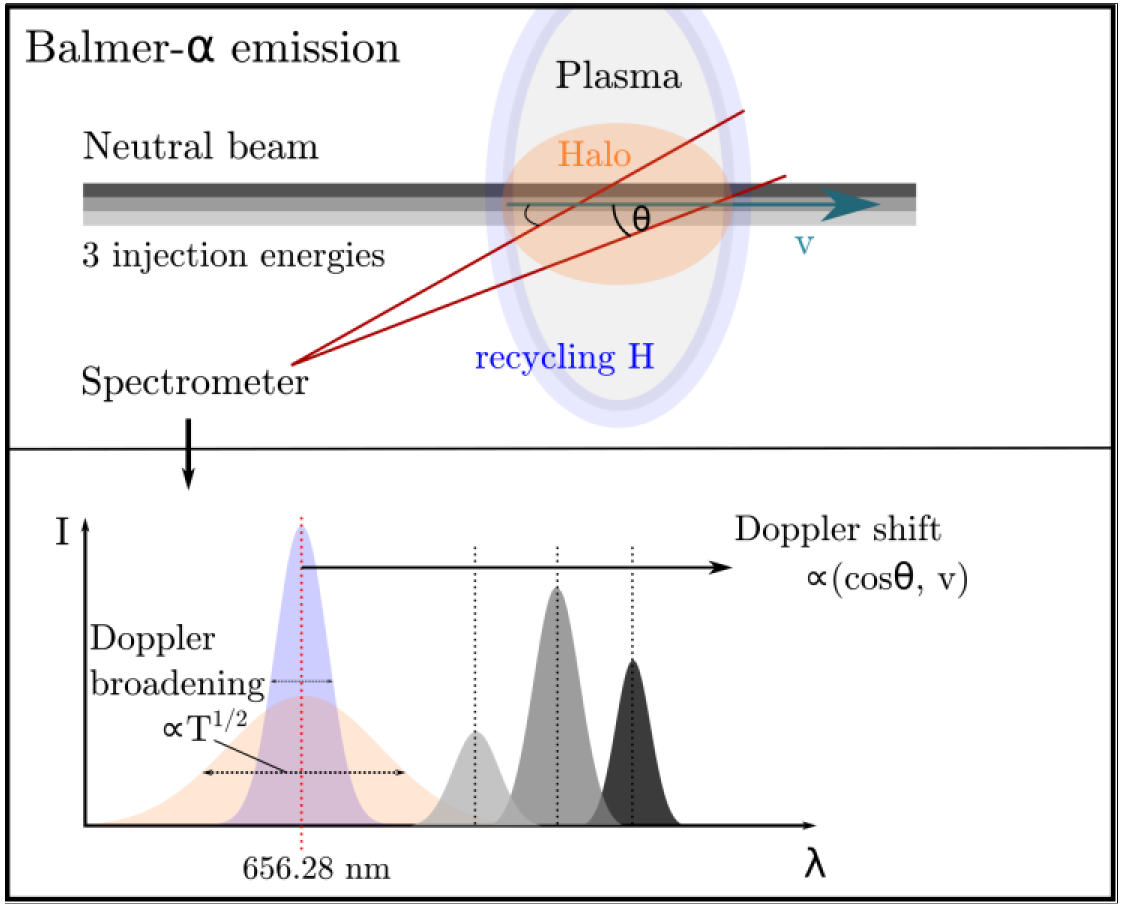
Neutral Beam Injection for heating at W7-X

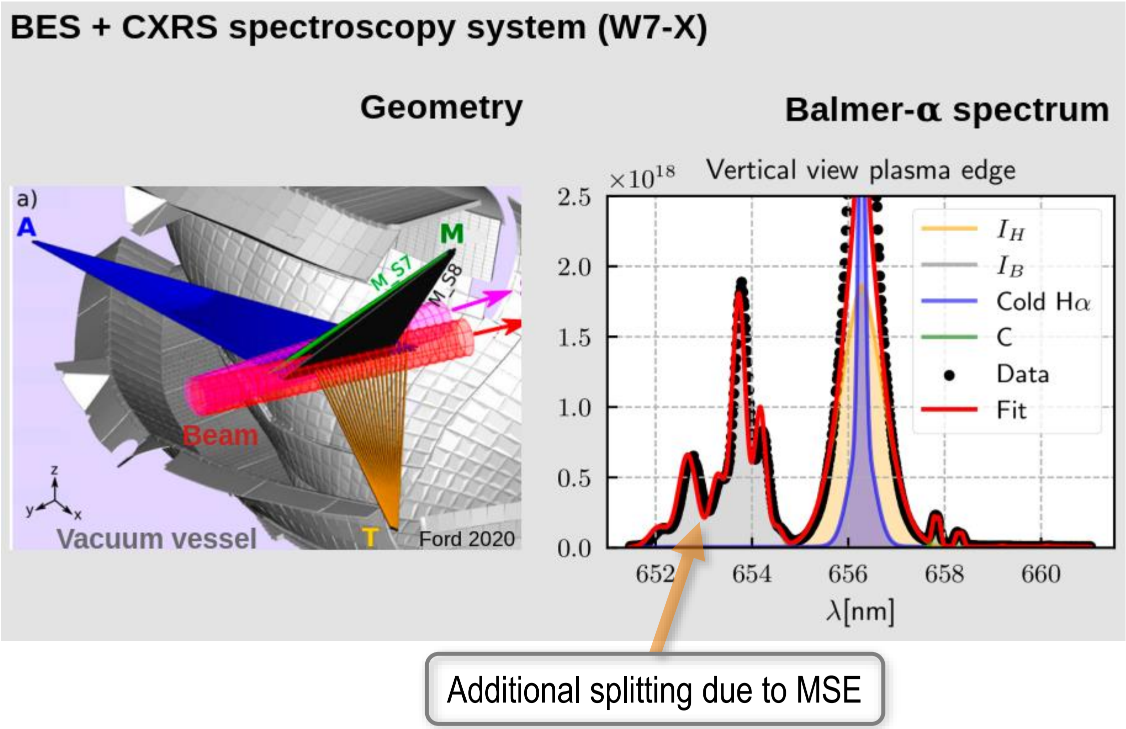
- 4 out of 8 planned beams commissioned so far
- Radial injection, 1.8 MW/source, 55 keV
- The source grid made up of pinholes → Several Gaussian beamlets used in the model





Spectral composition of beam emission





- Up to 54 lines of sight from three different ports used
- Complex spectra fitted well

S. Bannmann et al 2023 JINST 18 P10029

Model of beam particle emission

- Collisional-radiative model
  - Needed to model beam attenuation and emission
  - Track ground state + 5 excited states

$$\boxed{\frac{\mathrm{d}\mathbf{\Phi}(u)}{\mathrm{d}u} = \frac{1}{v_b}\mathbf{T}_{\mathrm{CR}}\mathbf{\Phi}(u)}$$

Neutral flux

$$\mathbf{T}_{CR} = \mathbf{T}_{CR}(T_e, T_i, n_e) = \begin{bmatrix} -L_1 & A_{21} & A_{31} & . & A_{k1} \\ E_{12} & -L_2 & A_{32} & . & A_{k2} \\ E_{13} & E_{23} & -L_3 & . & . \\ . & . & . & . & A_{ki} \\ E_{1k} & E_{2k} & . & E_{jk} & -L_k \end{bmatrix}$$

ColRad matrix

$$E_{ij} = n_e\langle\sigma_e^{(ij)}v\rangle + n_p\langle\sigma_p^{(ij)}v\rangle$$

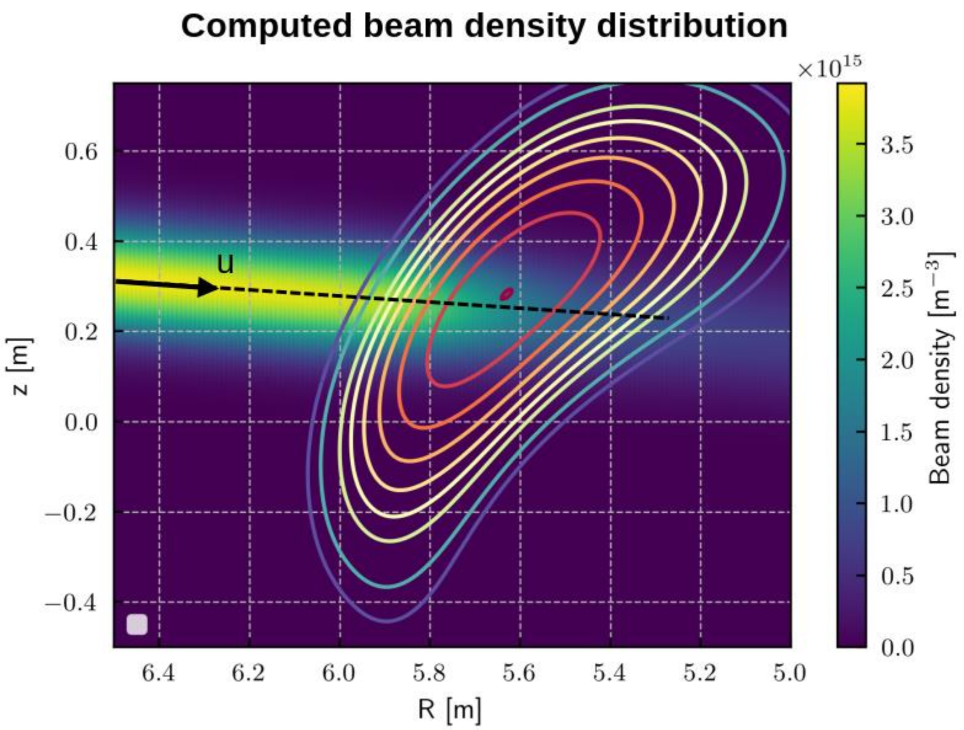
Excitation rate

$$L_i = \Delta_i + \sum_{m=i+1}^{k} E_{im} + \sum_{m=1}^{i-1} A_{im}$$

Total losses

$$\Delta_i = n_e\langle\sigma_e^{(iI)}v\rangle + n_p(\langle\sigma_p^{(iI)}v\rangle + \sum_{j=1}^{k}\langle\sigma_{\mathrm{CX}}^{(ij)}v\rangle)$$

Ionization losses



- Differential equations solved stepwise along each beamlet

Model of halo emission

- CX collisions of beam particles with background ions are source of the beam halo

Halo source term

$$S_{\mathrm{DCX}}^{(i)} = n_p \sum_{j=1}^{k} n_{\mathrm{B}}^{(j)} \langle \sigma_{\mathrm{CX}}^{(ij)} v \rangle$$

Halo density

$$\mathbf{n}_{\mathrm{Ha}} = (n_{\mathrm{Ha}}^{(1)}, ..., n_{\mathrm{Ha}}^{(i)}, ..., n_{\mathrm{Ha}}^{(k)})$$

- Halo particles undergo several CX collisions
- Travel ballistically between them → **Diffusion ansatz**

Diffusion ansatz

$$D_{\mathrm{CX}}^{(i)} = \frac{v_{\mathrm{th}}^2}{2n_{\mathrm{p}} \sum_{j=1}^{j_{\max}} < \sigma_{CX}^{(i \to j)} v_r >}$$

Assumptions

$$\begin{aligned} \partial_t \mathbf{n} &= 0 \\ \Delta_z, \Delta_\phi &<< \Delta_r \end{aligned}$$

- 1D diffusion equation coupled to CR model

$$-\nabla_r (D_{\mathrm{CX}}^{(i)} \nabla_r n_{\mathrm{Ha}}^{(i)}) = \sum_{j=1}^{k} T_{\mathrm{CR}}^{(ij)} n_{\mathrm{Ha}}^{(j)} + S_{\mathrm{DCX}}^{(i)}$$

Diffusion equation of state i

ColRad term couples diffusion eqs.!

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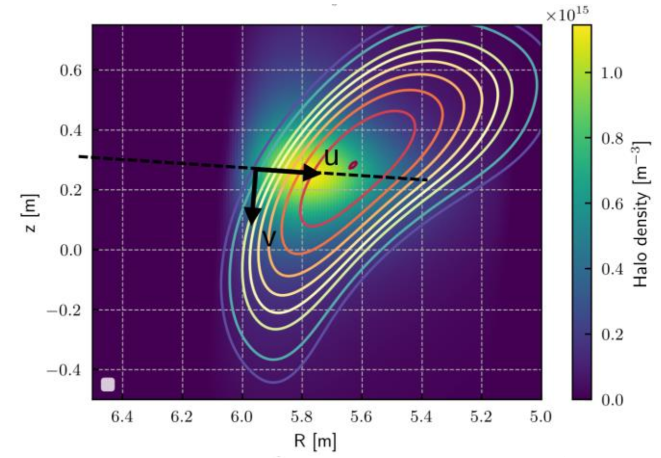
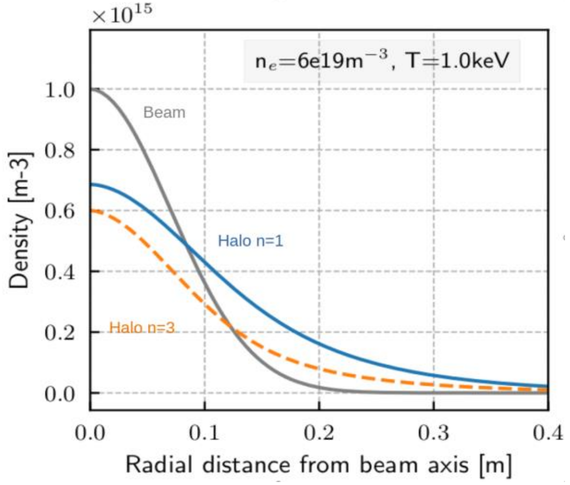
Computed halo density distribution





Highly complex model connecting n_e and T_i via various processes to measured H_α spectra

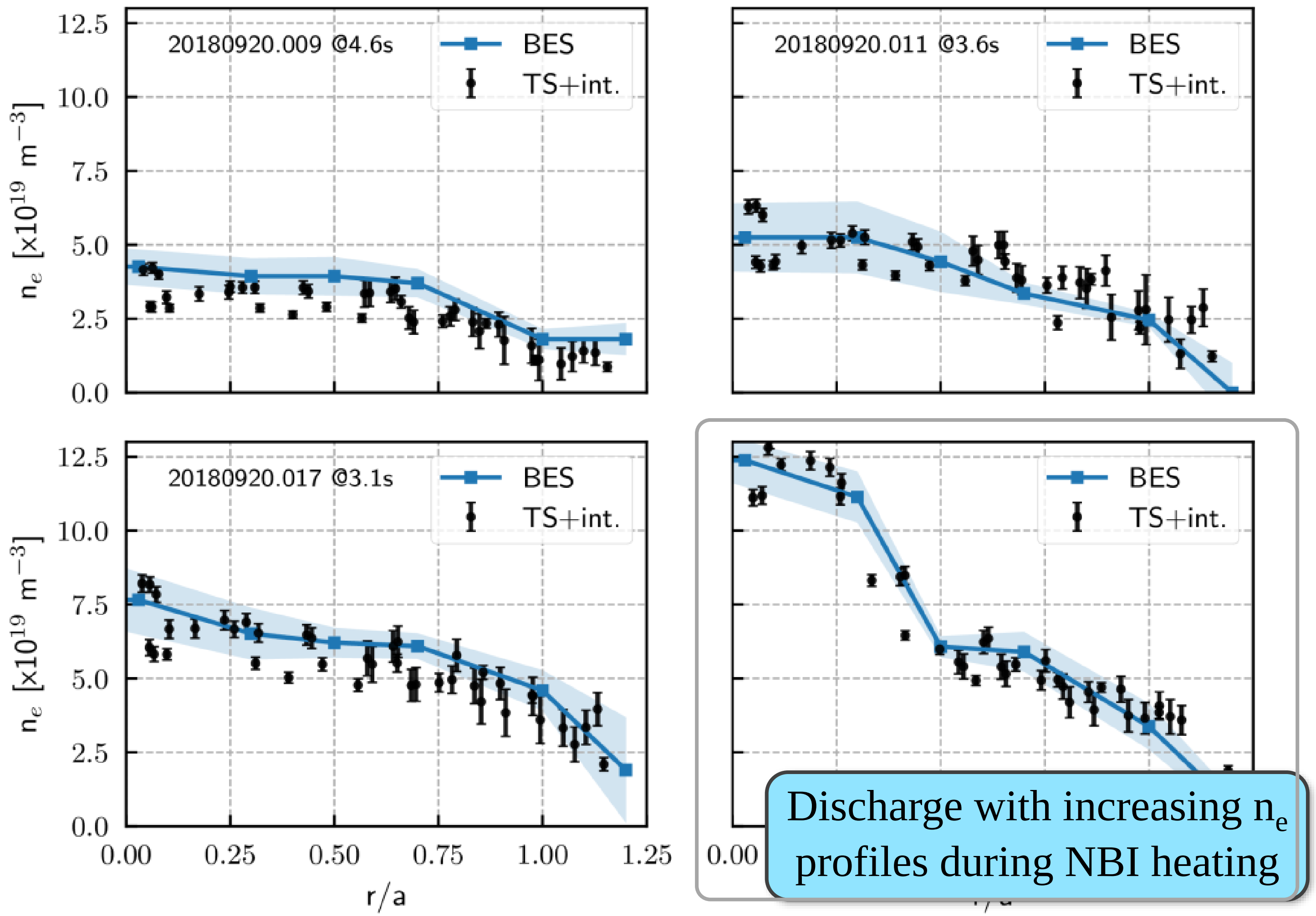
Beam emission spectroscopy – inference results

Bayesian MAP inference results

- Alignment of LOS – slightly adjusted
- Beam energy fractions and divergence – confirmed
- Vertical shift of the beam by ca. 5 cm
- Ion temperature profiles
- <u>Electron density profiles</u>

- Very good agreement found between ne profiles from BES and Thomson scattering

Electron density profile inference



S Bannmann *et al* 2024 *Plasma Phys. Control. Fusion* **66** 065001

Beam emission spectroscopy – Experimental anomalous particle transport

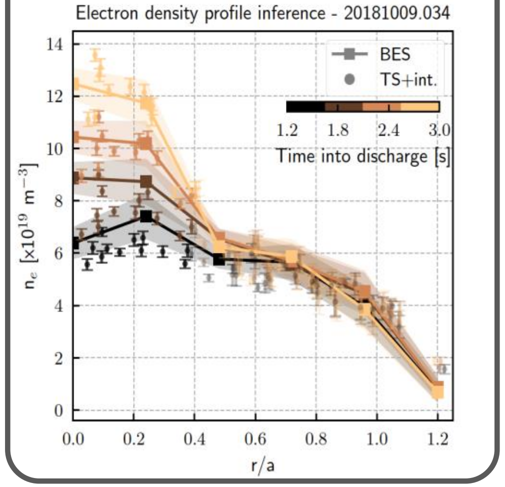
- W7-X was optimised for low neoclassical particle transport
- Turbulence is a major player
- Expected reduction of turbulent transport in scenarios with peaked n_e profiles
- Experimental confirmation: from inferred n_e profiles and NBI and recycling sources

$$\Gamma(r) = \left(\frac{dV}{dr}\right)^{-1} \int_0^r (S_{\mathrm{NBI}} + S_{\mathrm{RCY}} - \partial_t n)\frac{dV}{dr'}dr'$$

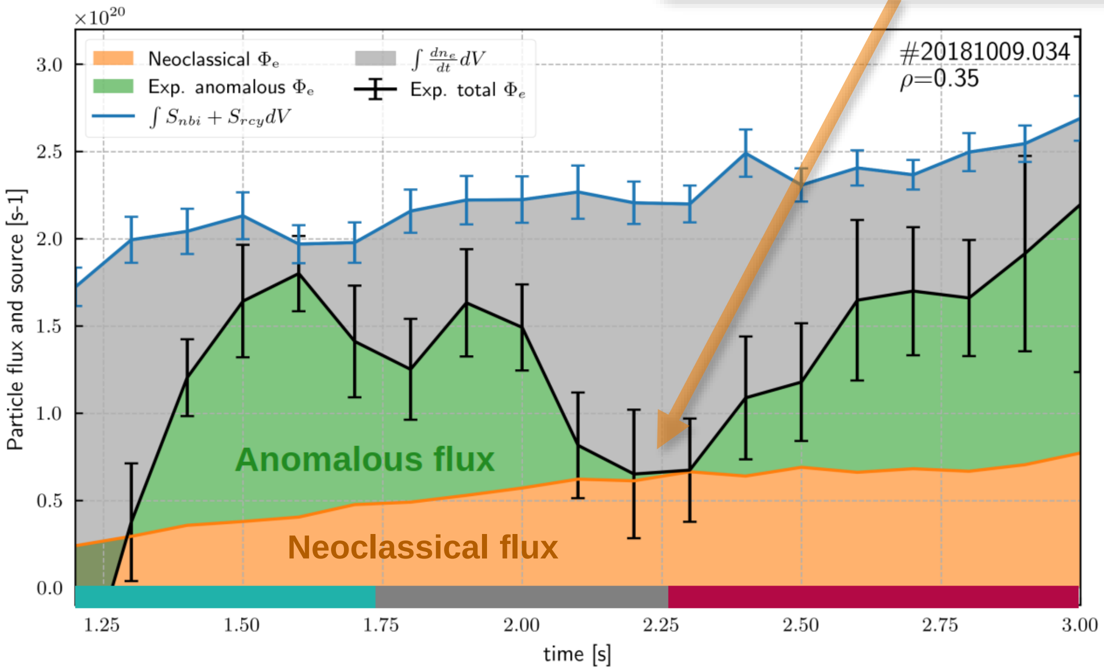
Particle source functions S [m-3s-1]

Change in density profile

Density build-up in pure NBI heating



Reduction of anomalous transport by peaked n_e profiles



S. Bannmann et al in Nucl. Fusion 64 106015

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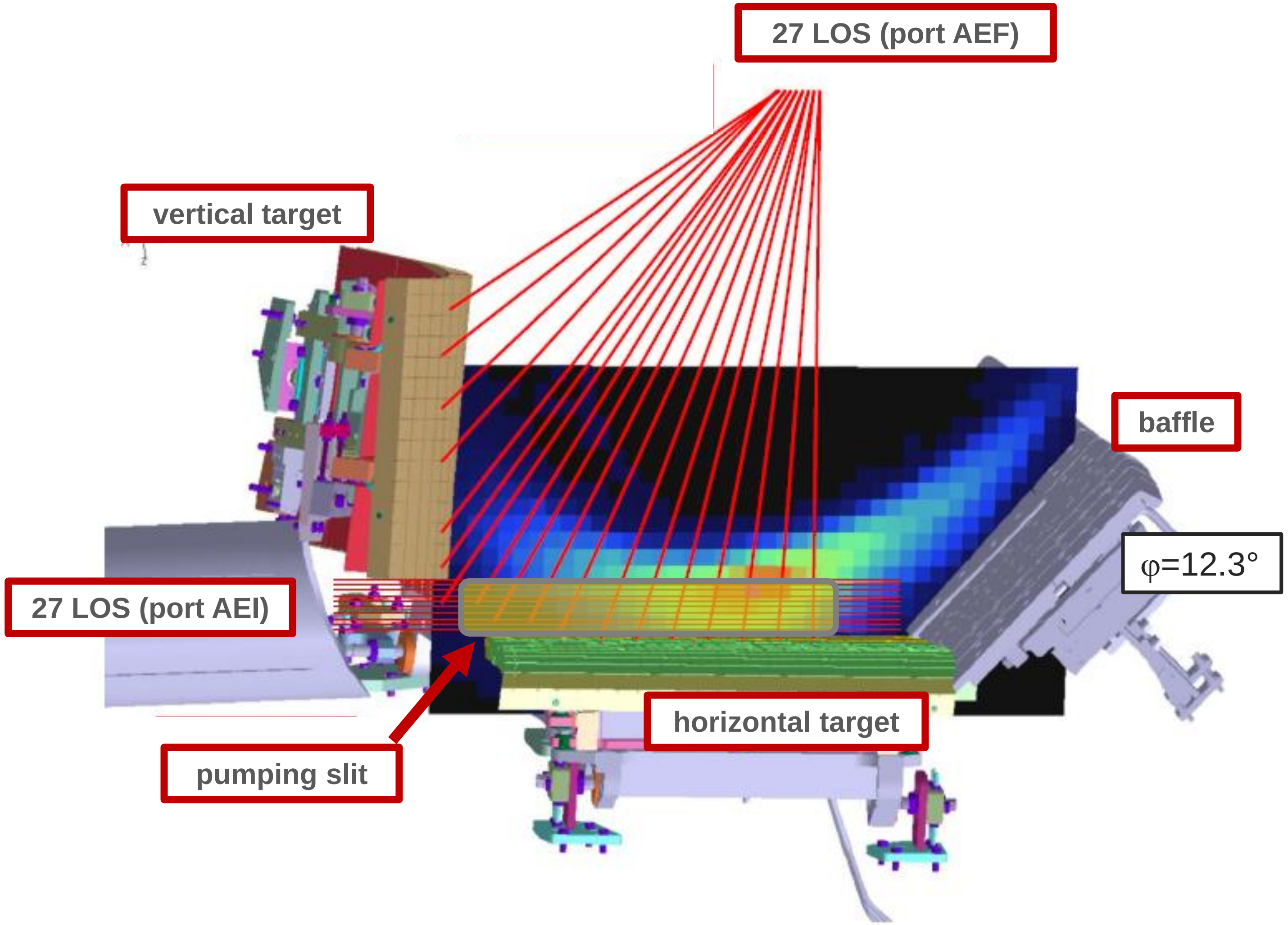
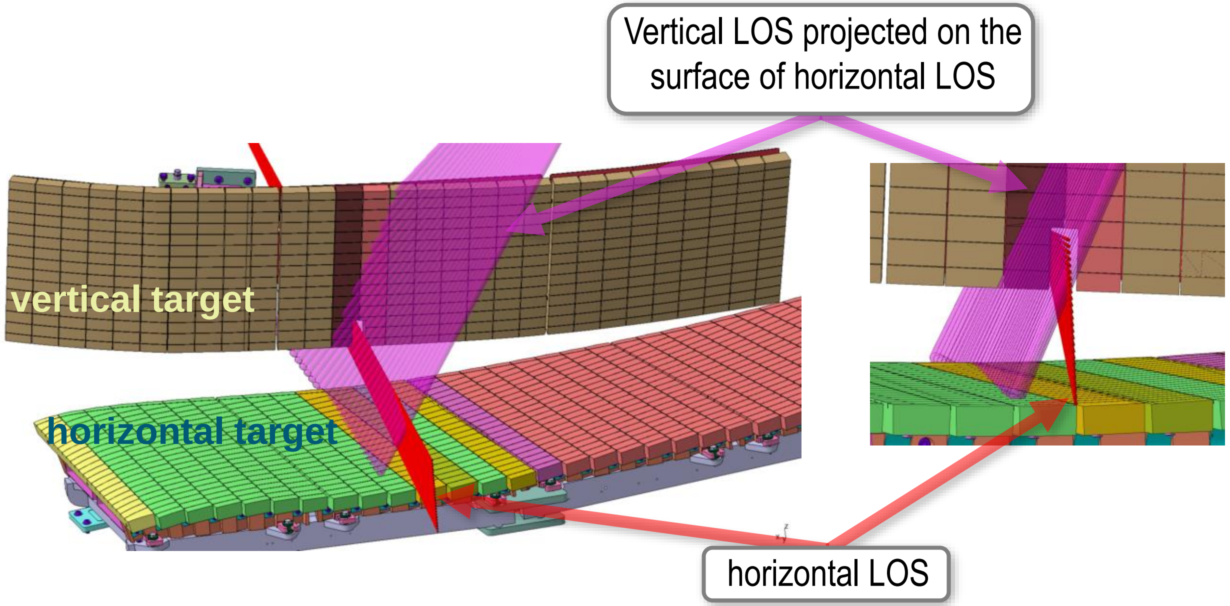
Divertor spectroscopy at W7-X

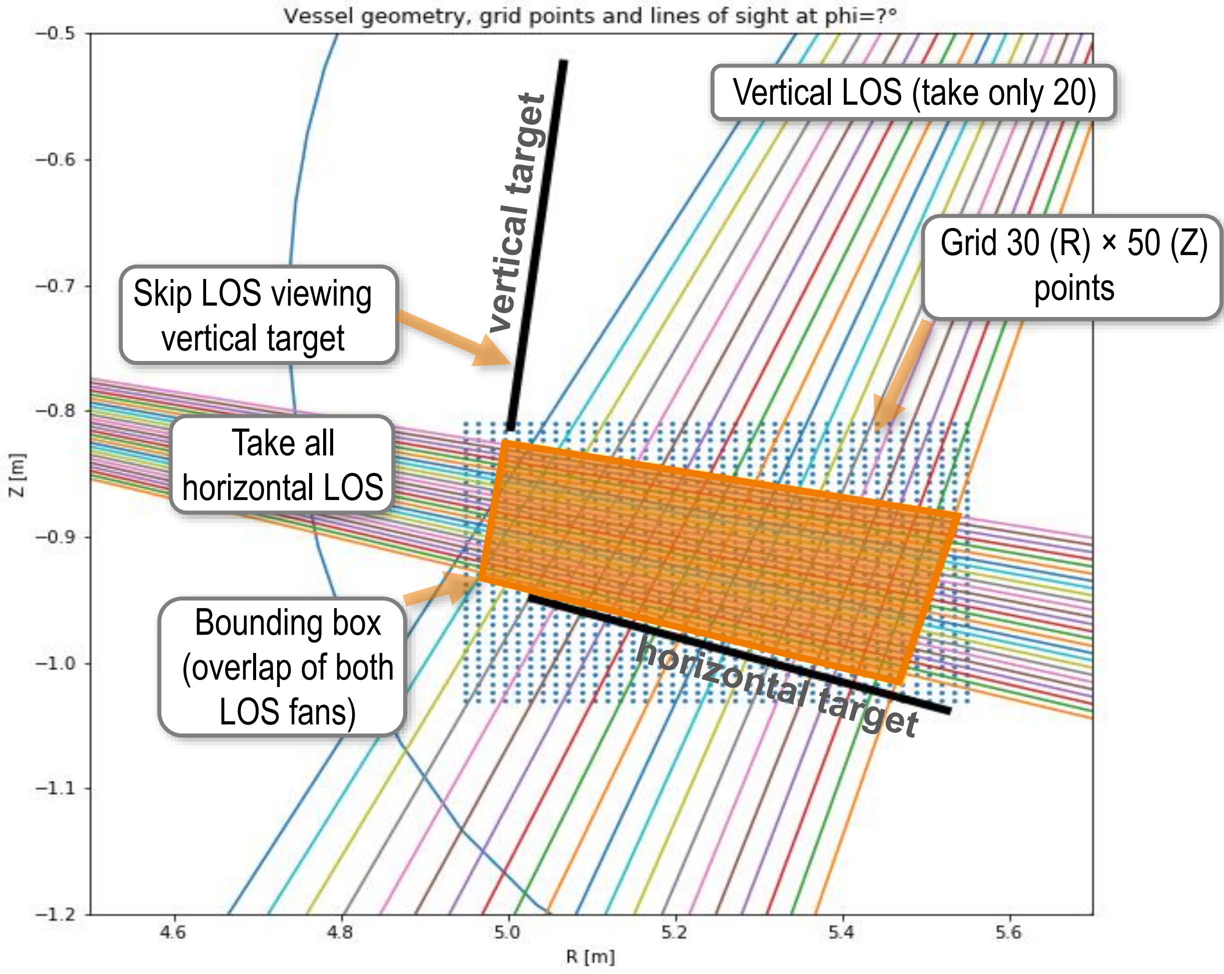
- 27 lines of sight in horizontal and vertical direction
- Same setup in one bottom (HM30) and one top (HM51) low iota divertor
- Light dispersed with several spectrometers with low, **middle** and high resolution attached
- Signals recorded with CCD cameras and IP160 spectrometers (f=160 mm) by Princeton Instruments



Geometry of the model

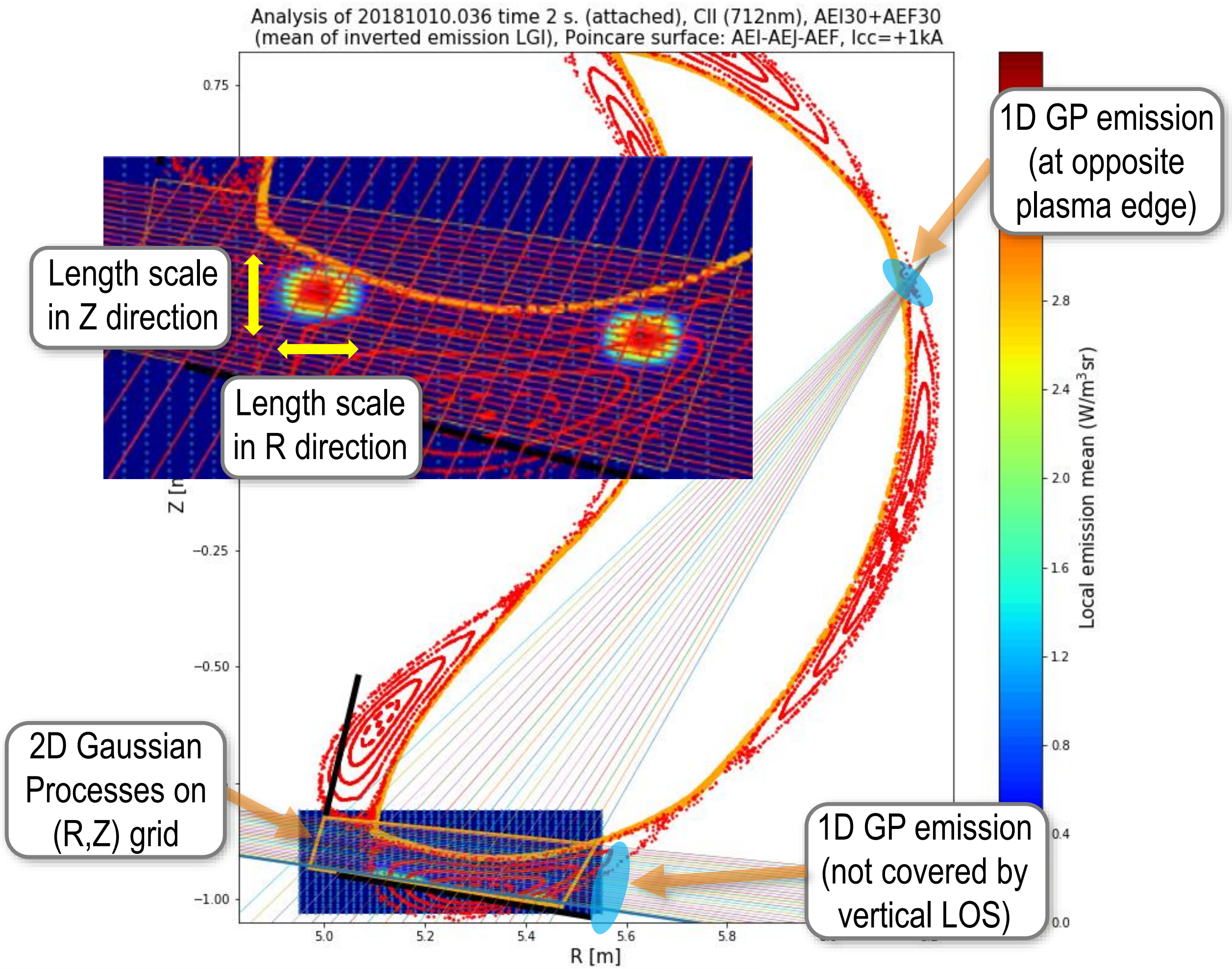
- Define a 2D grid of appr. 500 points where the horizontal and vertical LOS overlap
- Vertical and horizontal LOS fans tilted in toroidal direction
  - Project all LOS on one surface
  - Toroidal emission gradients are ignored





Emission model using Gaussian Processes

- 2D emission in divertor plasma modeled with non-parametric Gaussian Processes
- The only model (hyper)parameters
  - Correlation length scale in R and in Z direction
- The length scales are pre-optimised using the Bayesian Occam's razor principle
  - Reasonable optimum length scales obtained (Z: ~1 cm, R: ~5 cm)
- Two 1D emission zones added (not covered by 2D emission)
  - At horizontal target
  - At vertical port (AEF30)
- Additional assumptions on both emissions based on 3D plasma simulations could be added (e.g. shape of emission blob)

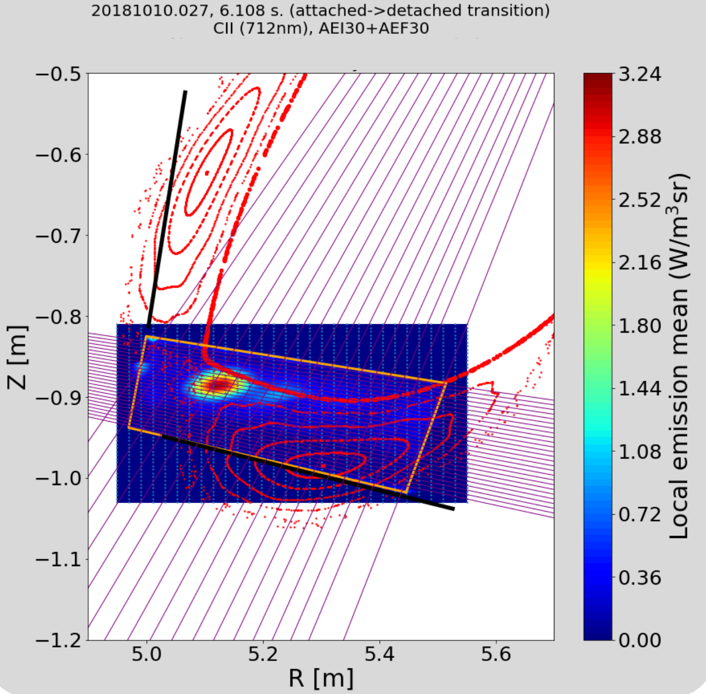


ill-posed tomographic problem with "incomplete" data set and uncertain outcome

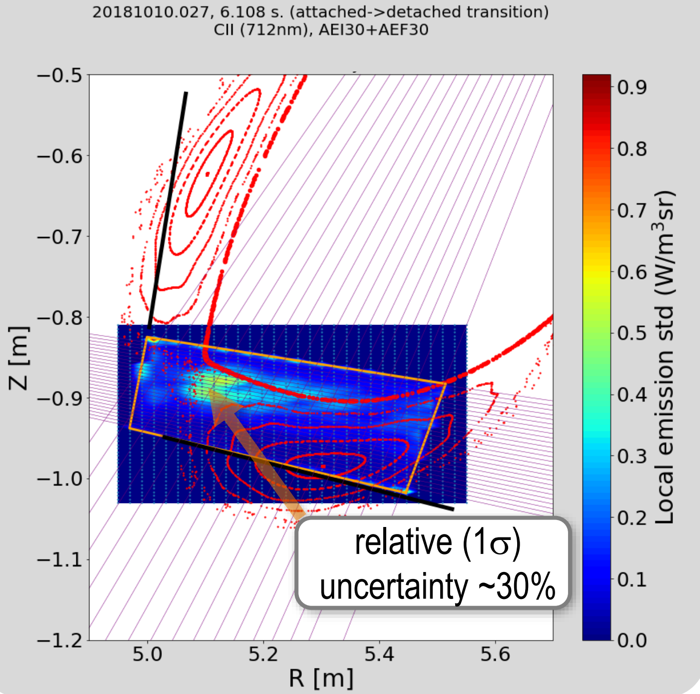
Inferred local emissions with uncertainties

- Assumed emission models are linear
  → Analytic solution possible (even when using Gaussian Processes for emission models)
- Truncation the emission to positive values necessary to avoid negative emissions
- Applied method
  - Linear Gaussian Inversion
  - With sampling from the truncated multivariate normal distribution of the emission
  - Inversion time ~1 min./time slice

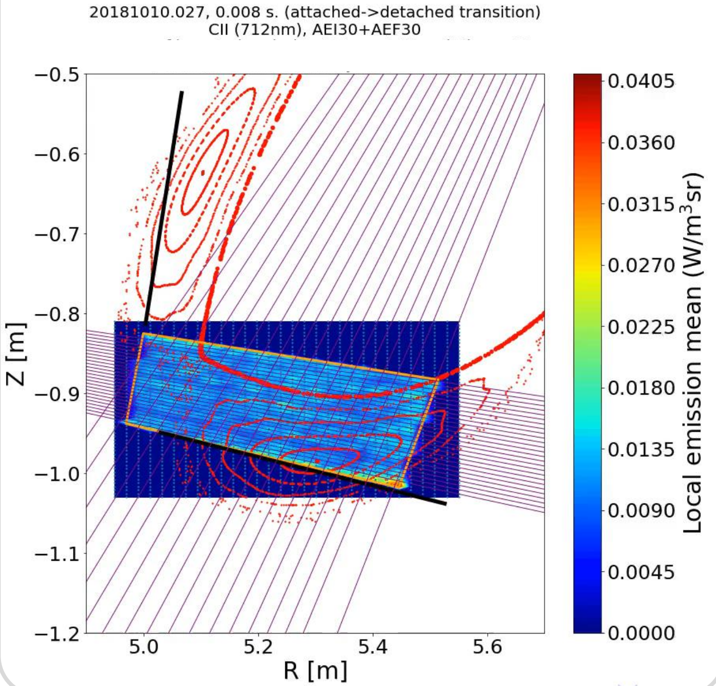
Mean of the 2D emission samples



St. deviation of the 2D emission samples

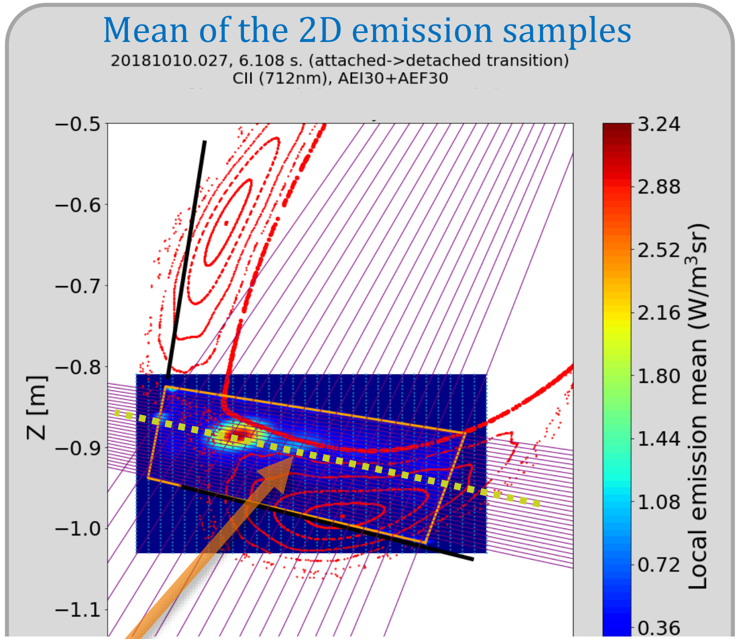


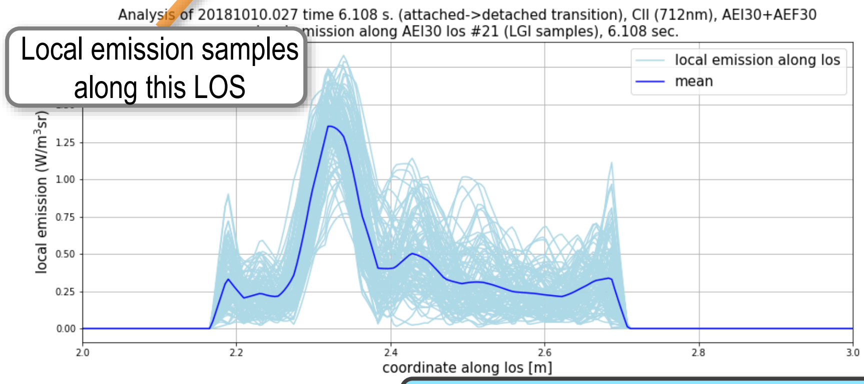
CII emission in transition to detachment



Inferred local emissions with uncertainties

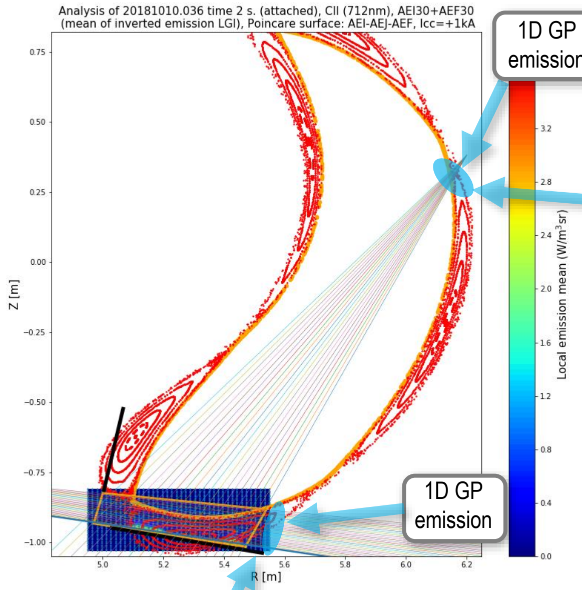
Local emission along LOS





Local emission samples along this LOS

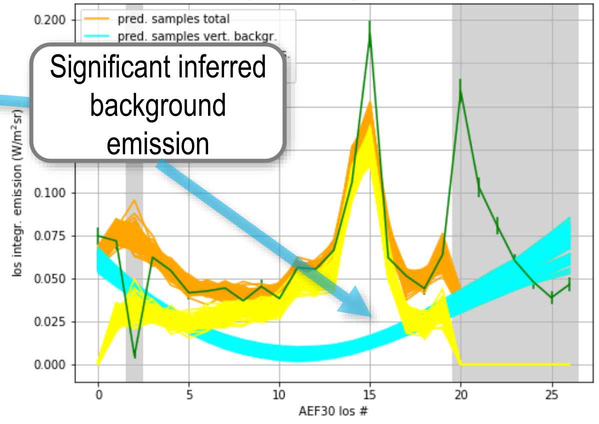
Samples of local 2D emission in divertor
→ Use for further analysis (including error propagation)



1D GP emission

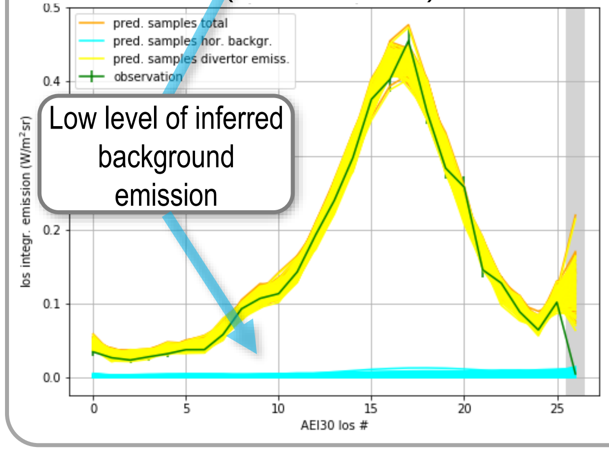
1D GP emission

Measured and predicted signals (vertical LOS)



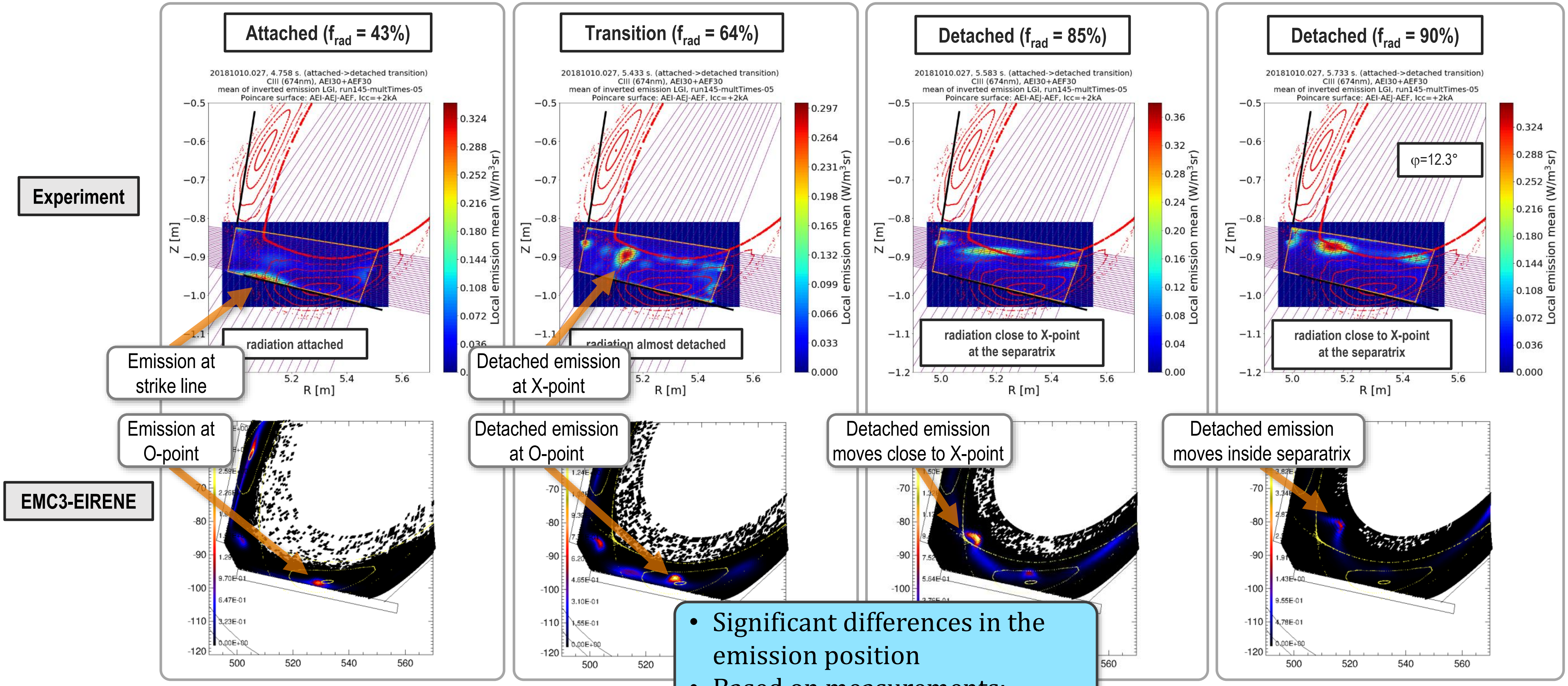
Significant inferred background emission

Measured and predicted signals (horizontal LOS)



Low level of inferred background emission

Inferred CIII emission compared to EMC3-EIRENE



- Significant differences in the emission position
- Based on measurements: further develop plasma models

M. Krychowiak et al., EPS 2021   Y. Feng et al, NF 2021

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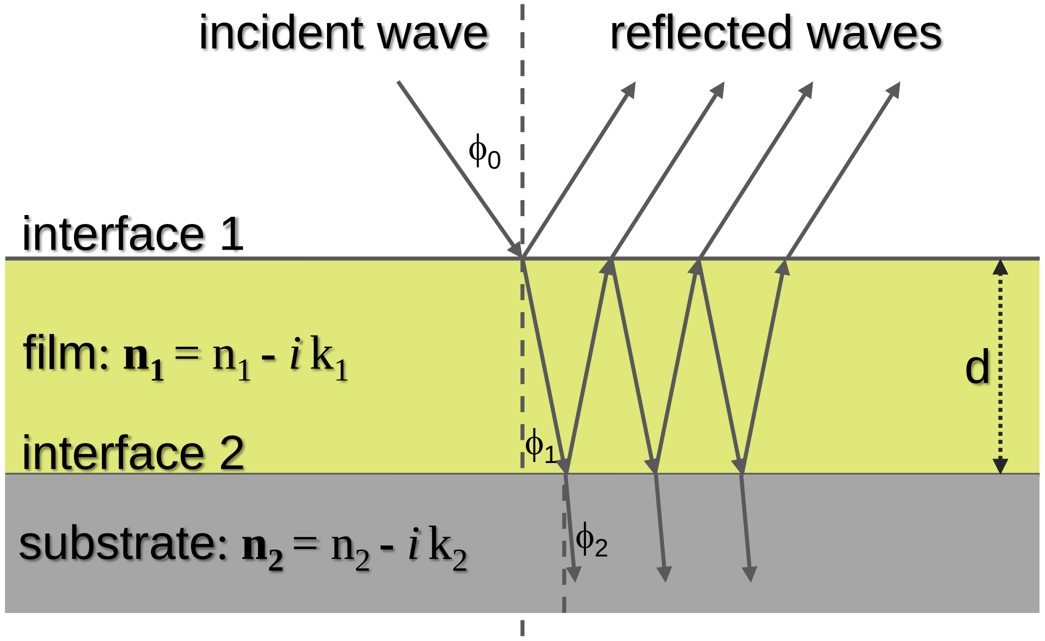
Principles of ellipsometry

- Electromagnetic wave reflected at an interface
- Multiple reflections at a thin layer → Interference patterns in reflected spectra



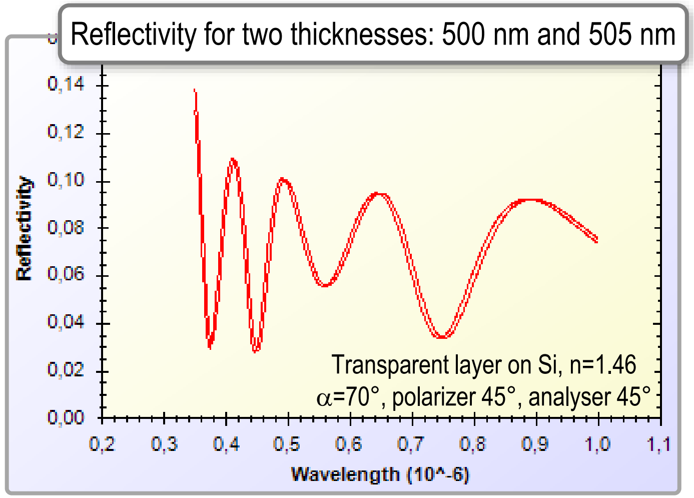
<u>Fresnel equations</u>

$$r^{\parallel} = \frac{n_0 \cos\phi_1 - n_1 \cos\phi_0}{n_0 \cos\phi_1 + n_1 \cos\phi_0}$$

$$r^{\perp} = \frac{n_0 \cos\phi_0 - n_1 \cos\phi_1}{n_0 \cos\phi_0 + n_1 \cos\phi_1}$$

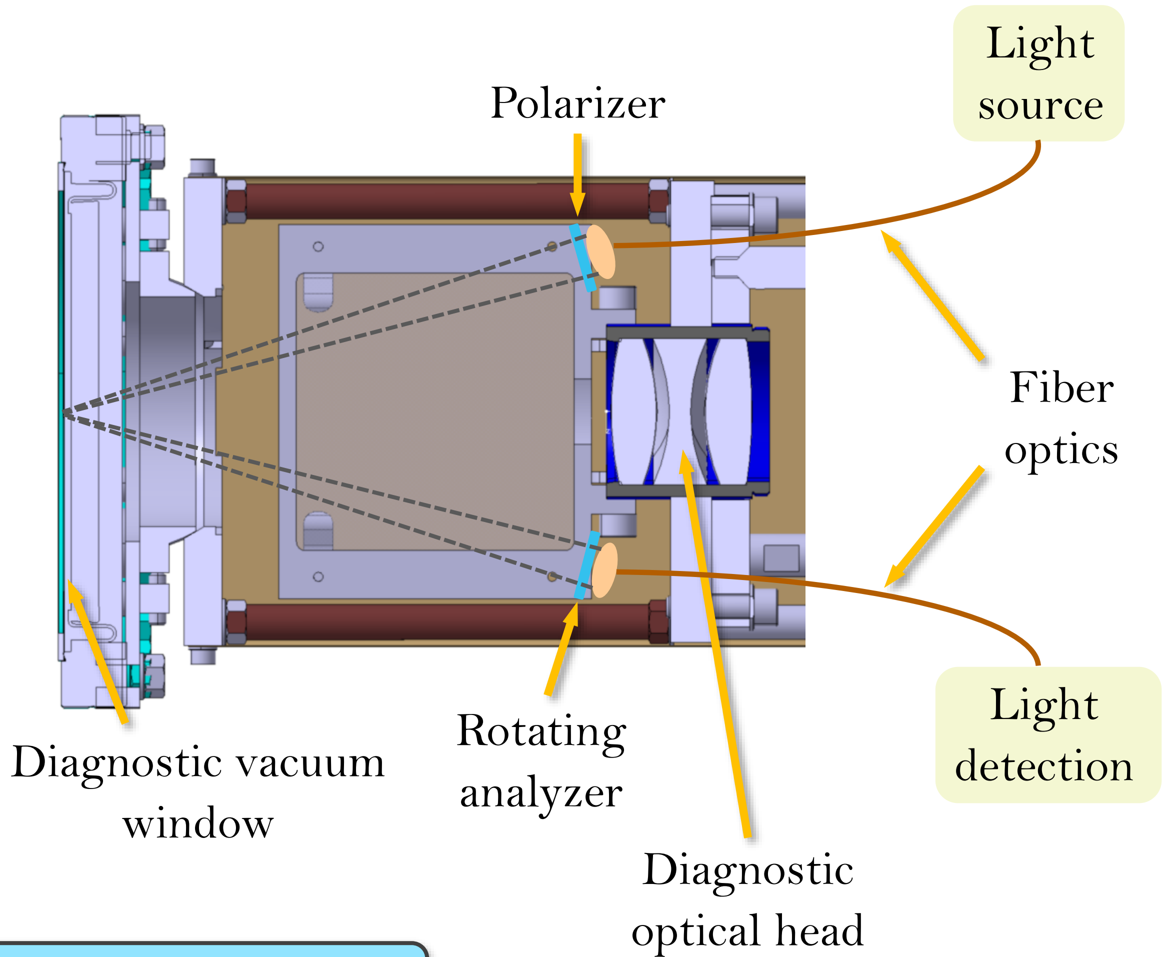
<u>Total reflection at thin single layer</u>

$$\boldsymbol{r} = \frac{\boldsymbol{r_1} + \boldsymbol{r_2} e^{-i\frac{4\pi}{\lambda} n_1 d_1}}{1 + \boldsymbol{r_1}\boldsymbol{r_2} e^{-i\frac{4\pi}{\lambda} n_1 d_1}}$$



Ellipsometry ideas for W7-X: vacuum window monitor

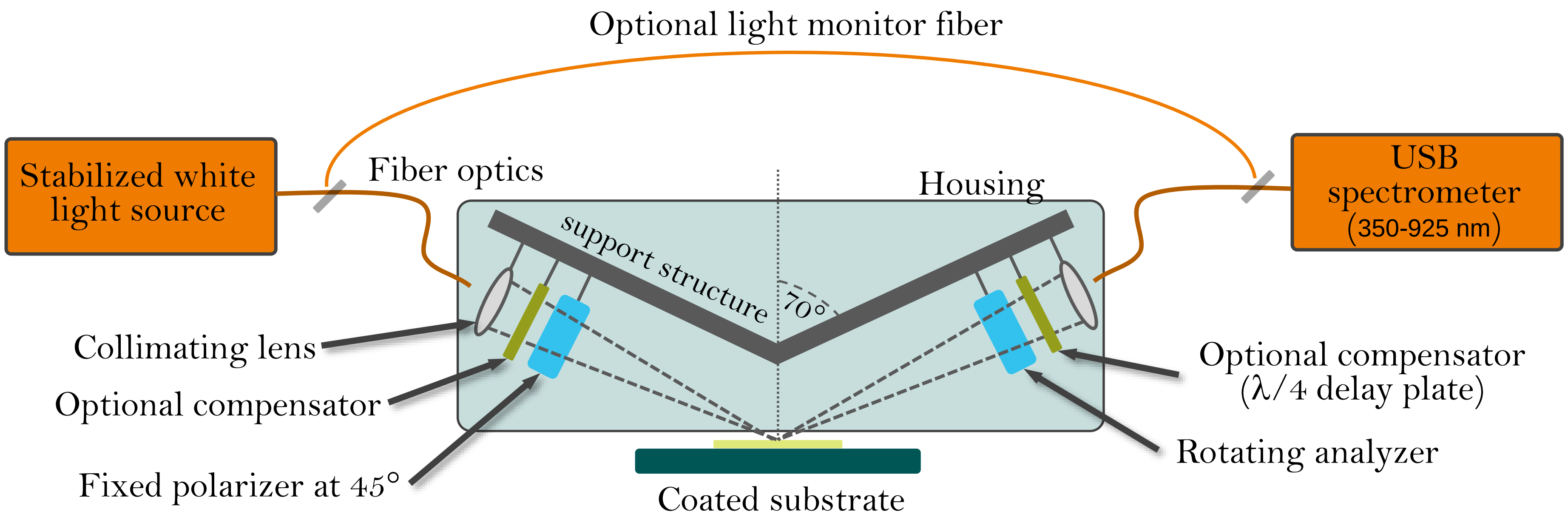
- During design phase of W7-X diagnostics
  - W7-X is a long-pulse machine (30 min.)
  - Coating of diagnostic windows expected
  - Attempt for in-situ monitoring of coatings
  - Self-made hardware setup
  - Compatible with considerable space restrictions
- “As simple as possible” ellipsometer
  - Detecting reflected intensities, relative (not absolute) phase delay
- Compensate simple hardware design by
  - Broad spectral range
  - Advanced data analysis to maximise the inference outcome



- W7-X behaves in a friendly manner towards vacuum windows
- The coating monitor was never built

Ellipsometry ideas for W7-X: thin layers at first wall components

- W7-X strongly involved in plasma wall interaction studies
- Hand-held ellipsometer for measurements of coating parameters in plasma vessel
- Various types of wall materials (steel, graphite, CFC, tungsten), roughness, shapes

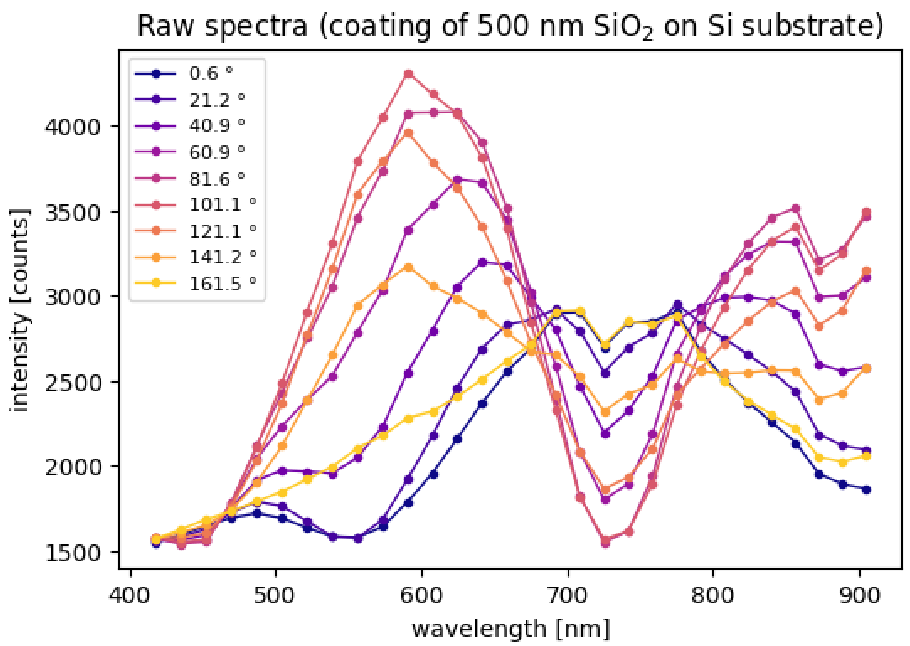


- Design is ready, device in manufacturing
- Planned to be used during actual opening phase (till Jan. 2026)

M. Krychowiak, Rev Sci Instrum. 2024 95(11)

Definition of spectral measurement set

- Full spectrum reflected at the layer
  - For different analyser angles (0-180°, e.g. in 20° steps) to sample the ellipticity of the polarised light
- Spectrum/intensity of incident light (at uncoated reference surface)
- Dark current

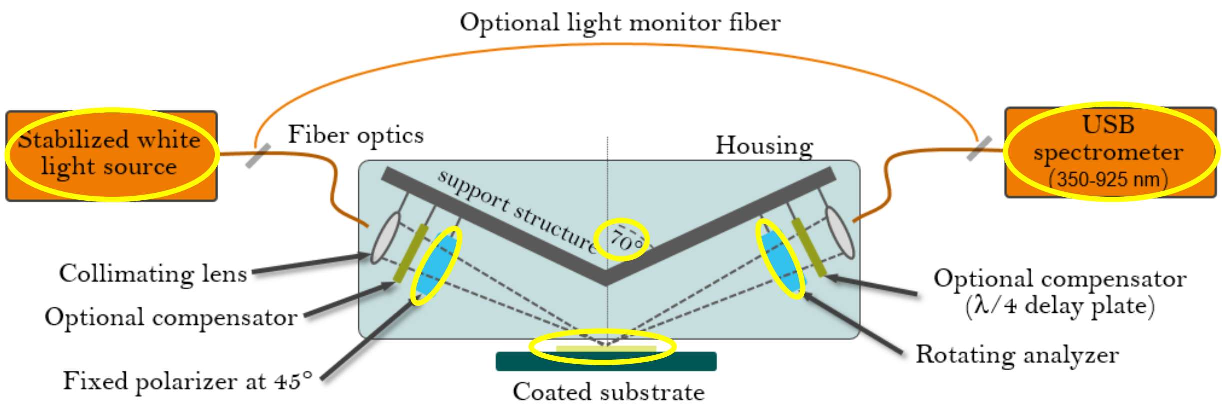


- Take only data points every ~15 nm
  - Speeds up the Bayesian analysis without loss of information
  - Number of data points can be optimised
- Raw spectra look very different for selected angles
  - Number and values of analyser angles can be optimised
- Wavelength range, exposure time, …

Apply the Bayesian diagnostic design using test and synthetic measurements to optimize
- The choice of hardware (light source, spectrometer, polarizer, ...)
- Definition of the data set to be acquired
- Mechanical tolerances (reflected spectra sensitive to geometry)

Bayesian model of the ellipsometer

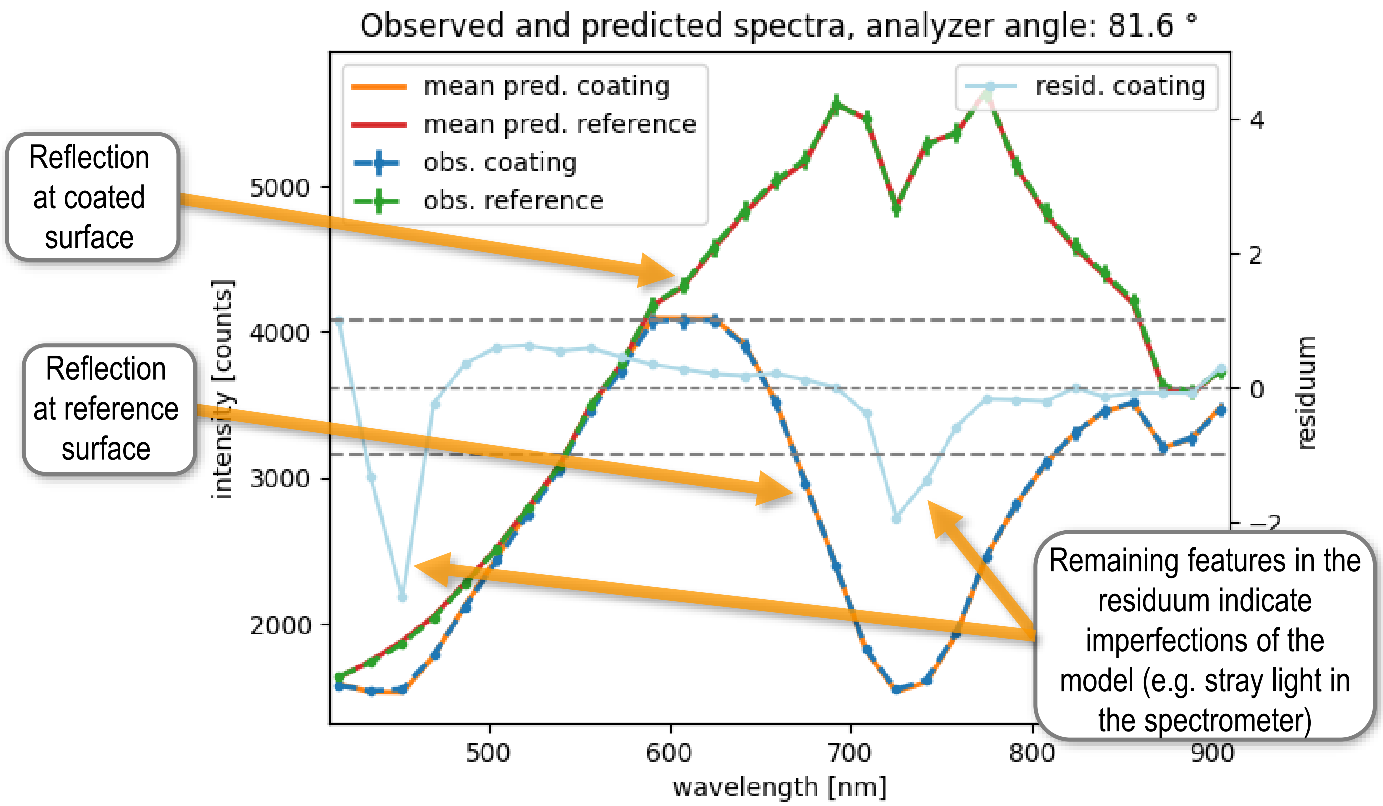
- Forward model for reflection of
  - Linearly polarised (p,s) light
  - At a single thin layer
  - Sampling the ellipticity of the reflected wave with the rotating analyser
- Free model parameters
  - Layer thickness, refractive index $n(\lambda)$ for some investigations
  - Geometric parameters: incident angle, polariser rotation angle, analyser rotation angles
  - Spectral shape of incident light (can change for longer measurements)
  - Linearity correction factors of the detector
- Non-linear model, apply MCMC to explore the posterior distribution



Ellipsometer model validation using test measurements

- Test measurements done using a lab setup
- A coating standard used with known parameters (492.4 nm of SiO_2 on Si substrate)
- Very good fits found for both spectra (also for all other analyser angles)

Coating standards (SiO_2 on Si)



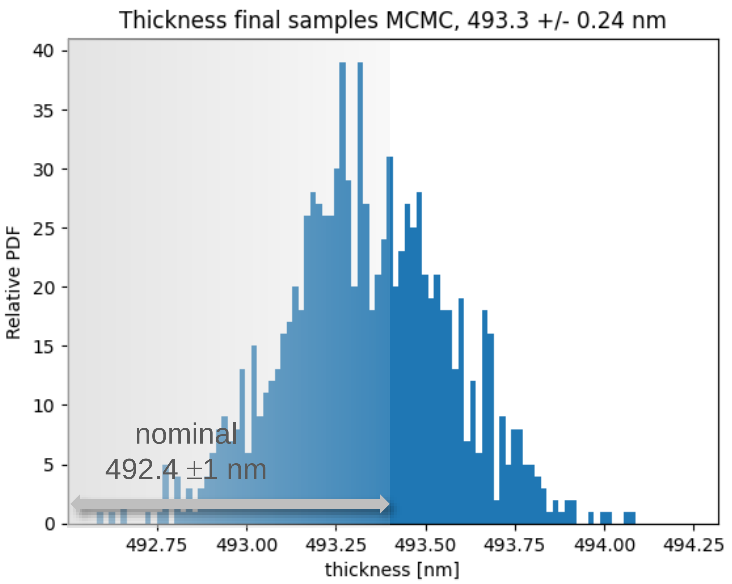
Inference of test measurements: calibration of geometric parameters

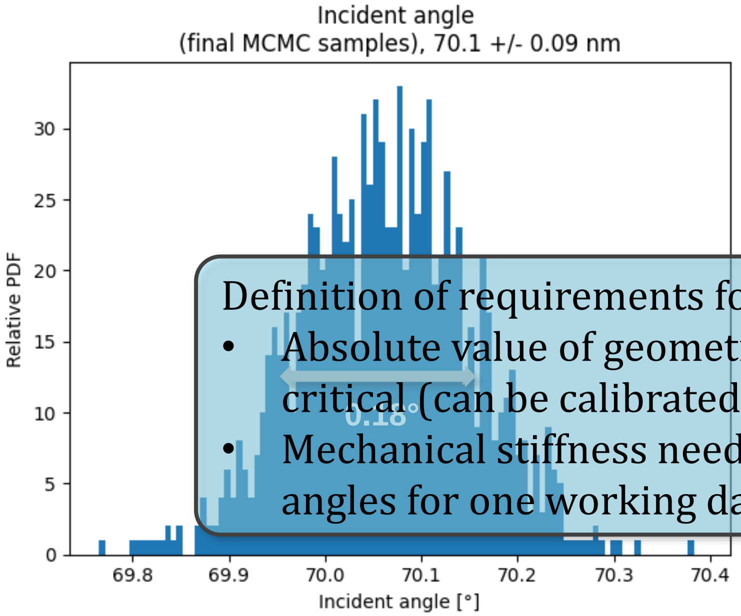
- Inference done for a set of measurements at different analyser angles (in 20° steps)
- The relative final error: 0.5×10^{-3}
- The nominal layer thickness reproduced very well
- Small shift of central wavelength likely due to imperfections of the model

- Prior for incident angle: normal distribution, 70° ±3°
- Final result: 70.1° ±0.09°
- Similar accuracies (of ~ ±0.15°) obtained **for all geometric parameters**

→ Ellipsometry is sensitive to geometric parameters

→ All angles can be precisely calibrated using the coating standard



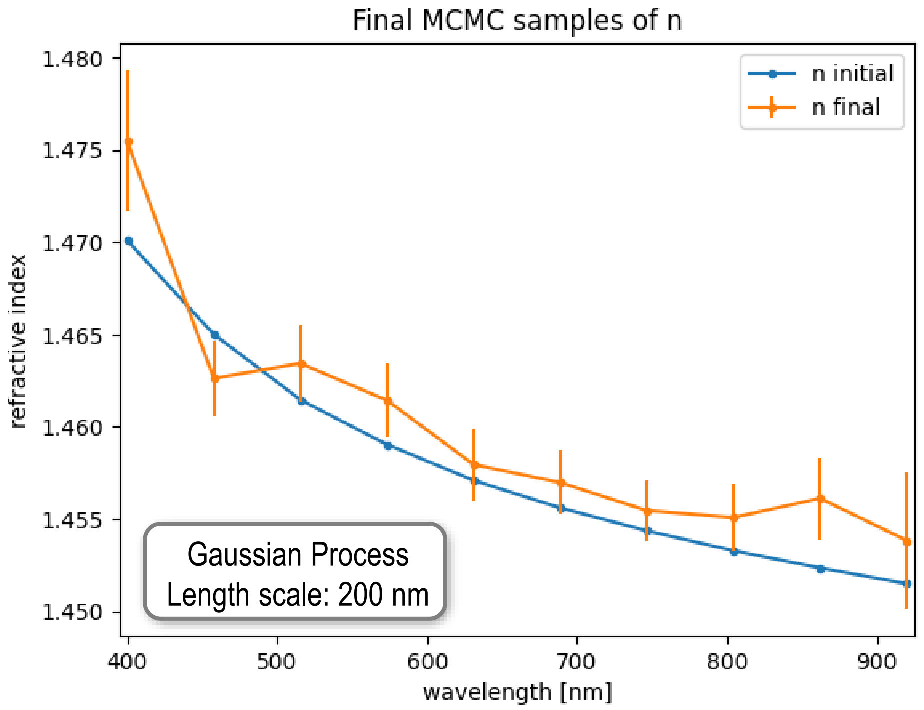


Definition of requirements for mechanical design
- Absolute value of geometric parameters not critical (can be calibrated)
- Mechanical stiffness needs to ensure constant angles for one working day within e.g. ±0.1°

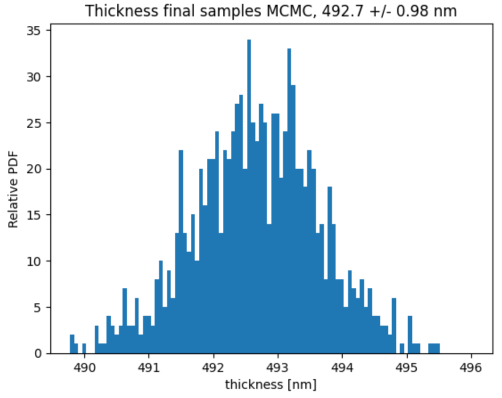
Inference of test measurements: fitting refractive index

- In last example refractive index *n(λ)* was assumed as known
- Fit *n(λ)* assuming geometric parameters: nominal values well reproduced

→ Potential of the method to derive even *n(λ)* at least in some cases



Uncertainty of thickness increased from ±0.25 nm to ±1 nm still reasonably small



Bayesian diagnostic design with synthetic data

- In order to cover larger parameter space the diagnostic design can be done using synthetic (noisy) data

Change of the model	Layer thickness uncertainty
Assume lowest expected uncertainty of geometric parameters: ±0.1°	very low (use of perfect model) ±0.05 nm
Add refractive index n = f(λ) to free parameters	considerably increased: ±0.8 nm (n: ±0.001)
Increase 5x (up to ±0.5°) the uncertainty of: - incident angle - polarizer angle - all 9 analyzer angles	further increased: ca. ±1.1 nm

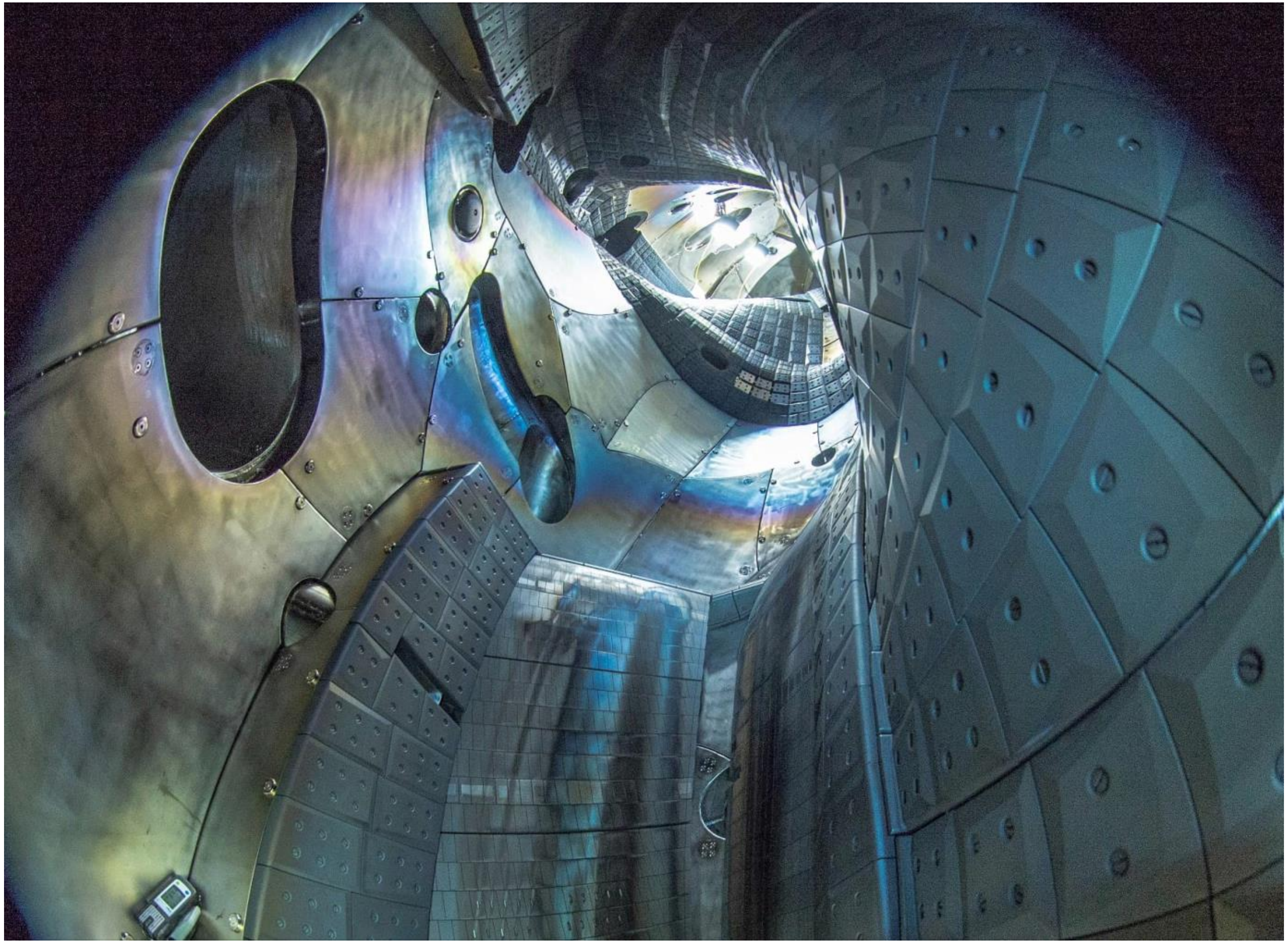
Counter measures to reduce thickness uncertainty	
Doubled number of data points (every 7 nm)	±1.05 nm
Extended wavelength range 350-1200 nm	±1.08 nm
Doubled number of analyzer angles (10° steps)	considerably reduced: **±0.50 nm**

- Bayesian diagnostic design using synthetic data has a large potential to optimise hardware selection, define mechanical tolerances etc.
- Needs further analysis with other substrate materials (graphite, ...), not transparent layers, multi-layers, ...

Summary

- Three examples of Bayesian data analysis at W7-X discussed
- *Complexity*: Inference of n_e profiles and particle sources from BES
  - Experimental confirmation of reduced turbulent particle transport in plasmas with density gradients
- *Model (hyperparameters) optimisation*: Gaussian Process Tomography of carbon radiation in divertor plasma
  - Ill-posed problem with “incomplete” measurements
  - Pre-optimisation of emission correlation length scales was used
  - Reasonable behaviour of carbon emission in transition to detachment
  - Significant differences in emission position in comparison to EMC3-EIRENE modelling
- *Bayesian diagnostic design*: Ellipsometry to measure parameters of thin coatings at first wall components
  - Bayesian inference of test and synthetic data helped to define hardware components (light source, spectrometer) and mechanical tolerances
  - A hand-held ellipsometer in manufacturing for measurements in the plasma vessel this year

Thank you for your attention



View into the plasma vessel of W7-X
Courtesy. C. Biedermann, G. Wurden