MAX-PLANCK-INSTITUT
FÜR PLASMAPHYSIK

Bayesian inference of plasma and impurity parameters with spectroscopy

Related document:
D1.1 – First iteration of the report on the real-time analysis model for the 55.E6 VSRS diagnostic (ITER_D_6MJ4QZ v1.3)
D1.2 – Second iteration of the report on the real-time analysis model for the 55.E6 VSRS diagnostic (ITER_D_6MJ7EM v1.1)
D1.3 – Report on the real-time analysis model for the 55.E6VSRS diagnostic (ITER_D_6MHN3J v1.1)
D2.1 – First iteration of the report on the full Bayesian analysis model for the 55.E6 VSRS diagnostic (ITER_D_6MJ7CL v1.1)
D2.2 – Second iteration of the report on the full Bayesian analysis model for the 55.E6 VSRS diagnostic (ITER_D_6MJ84Q v1.0)
D3.1 – First iteration of the report on the integrated Bayesian analysis model for multiple spectroscopic diagnostics (ITER_D_6MJ72F v1.0)

Presented by Sehyun Kwak on the behalf of the Contributors

EUROfusion

This work has been carried out within the framework of the EUROfusion Consortium, funded by the European Union via the Euratom Research and Training Programme (Grant Agreement No 101052200 — EUROfusion). Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the European Commission. Neither the European Union nor the European Commission can be held responsible for them.

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Content

- Introduction
- Development of the Z_{eff} model for applications at W7-X
- Adaptation of the model for the Visible Spectroscopy Reference System at ITER
- Z_{eff} inference from the full spectrum and automated spectral line extraction

Plasma diagnostic modelling in nuclear fusion experiments

- Key parameters:
  - Particle densities: n_e, n_i
  - Particle temperatures: T_e, T_i
  - Plasma radiation, Z_eff, etc.

- Diagnostic observations of various physical processes:
  - Thomson scattering $\leftarrow n_\mathrm{e}, T_\mathrm{e}$
  - Interferometry $\leftarrow n_\mathrm{e}$
  - Beam emission spectroscopy $\leftarrow n_\mathrm{e}, T_\mathrm{i}$, etc.
  - Passive spectroscopy (bremsstrahlung, charge exchange) $\leftarrow Z_\mathrm{eff}, T_\mathrm{i}$, etc.
  - Soft X-rays, bolometry, etc.

Plasma diagnostic modelling in nuclear fusion experiments

- Data analysis: constructing an inverse function f^{-1} for an individual diagnostic (inverse problem)

$$D \xrightarrow{f^{-1}} H$$

D: Thomson scattering spectra, interference patterns, etc.
H: $n_{\mathrm{e}}, T_{\mathrm{e}}, T_{\mathrm{i}}$, etc.

- Challenges:
  - Problem might be not or only partially *invertible* (e.g., ill-posed)
  - Uncertainty quantification
  - Data fusion: merging diverse observations to obtain a consistent solution
  - Model selection: avoiding over- or under-fitting
  - Additional practical concerns: maintenance, debugging, etc.

Bayesian modelling within the Minerva framework

- Constructing a predictive forward model (forward problem) $f(H)$
  - The model predicts observations given specific parameters.

- Bayesian probability: the language of uncertainty (and model comparison)
  - The state of knowledge of model parameters can be explicitly represented as a probability distribution both prior to and posterior to observations, allowing uncertainties to be quantified without any loss of information.

- Bayes' theorem: the posterior distribution for any combination of observations

- Graphical model: unfolding the complexity of the model in which *everything* is declared.
  - Model assumptions (regularization), systematic parameters, and other aspects are clearly defined in the model and easily accessible through graphical representation, facilitating maintenance, debugging, reproducibility, etc.

J. Svensson, A. Werner et al. International Symposium on Intelligent Signal Processing-WISP (2007)

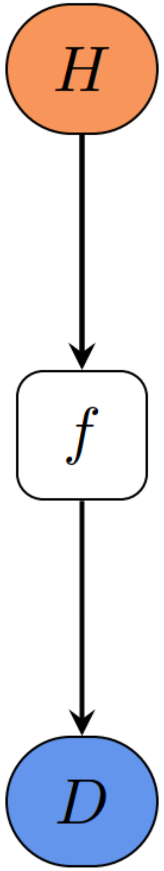
Bayesian modelling within the Minerva framework

- Defining the prior state of the system: $P(H)$ $(H\!: n_\mathrm{e}, T_\mathrm{e}, \text{etc.})$
  - Declaring model assumptions based on underlying physics and/or ad-hoc regularisation.

- The predictive distribution over observations $P(D|H)$ captures the physical processes occurring during experiments, defined by the forward model $f(H)$.

- Once the observations are available, we can update $P(H)$ to the posterior state $P(H|D)$ by Bayes' theorem:

$$P(H|D) = \frac{P(D|H)P(H)}{P(D)}$$



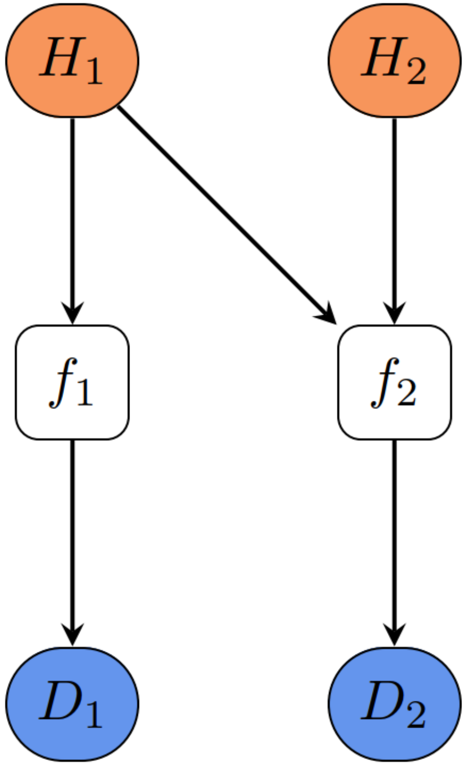
Bayesian modelling within the Minerva framework

- Data fusion: straightforward in Bayesian modelling
  - Example case: two unknown parameters H_1 and H_2 and two different observations D_1 and D_2. D_1 depends on H_1 and D_2 depends on H_1 and H_2:

$$P(H_1, H_2|D_1, D_2) = \frac{P(D_1, D_2|H_1, H_2)P(H_1, H_2)}{P(D_1, D_2)}$$

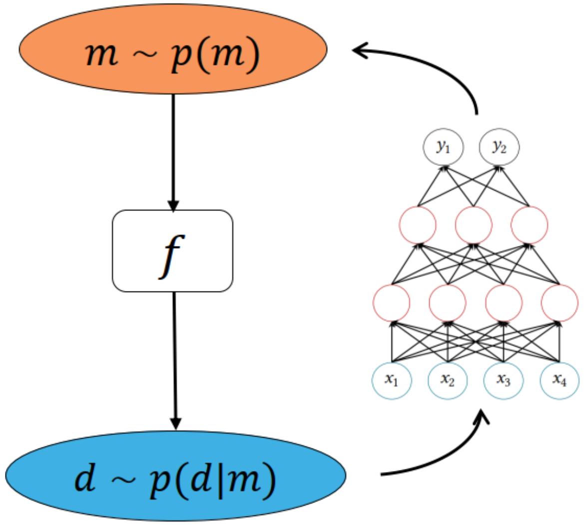
$$= \frac{P(D_1|H_1)P(D_2|H_1, H_2)P(H_1)P(H_2)}{P(D_1)P(D_2)}$$

  - Can be generalised for any number of parameters and observations.

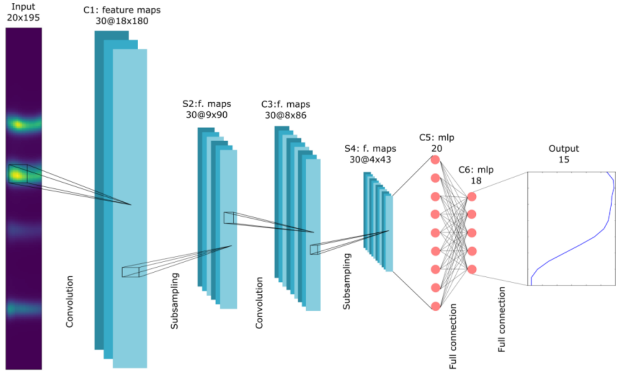


Deep learning surrogates within the Minerva framework

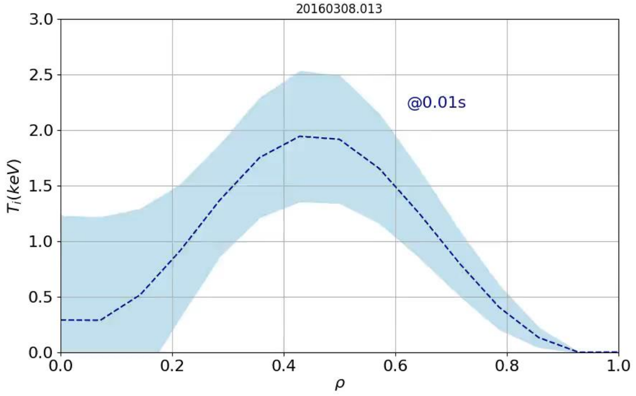
- Main obstacle of Bayesian inference: inversion time
- Can be overcome by accelerating Minerva models through the use of deep learning surrogates:
  - Training a deep learning model with synthetic data generated by the Minerva models
- Applicable to any Minerva model for fast inference ($\approx 100\ \mu s$)
- Accelerated applications:
  - X-ray imaging spectrometers (T_i profiles)
  - Single LoS Z_eff
  - VMEC equilibria
  - Lithium beam diagnostics (n_e profiles)



A. Pavone, Machine learning approximation of Bayesian inference in nuclear fusion PhD thesis



A. Pavone et al. »Neural network approximation of Bayesian models for the inference of ion and electron temperature profiles at W7-X«. In: *Plasma Physics and Controlled Fusion*, Vol. 61.7 (May 2019), page 075012. DOI: 10.1088/1361-6587/ab1d26.



Minerva models and applications

Minerva framework from
Seed eScience Research

W7-X diagnostics

- Interferometers / Thomson scattering [S Kwak et al 2024 Nucl. Fusion 64 106022]
- Helium beam diagnostics [E. Flom et al. Nucl. Mat. and Energy 33 101269]
- ECE [U. Höfel PhD Thesis TU Berlin 2020]
- X-ray spectroscopy [A. Langenberg et al 2021 Nucl. Fusion 61 116018] + Neural network fast surrogate [A Pavone et al 2019 Plasma Phys. Control. Fusion 61 075012]
- Z_{eff} profiles [S Kwak et al. Rev. Sci. Instrum. 92, 043505 (2021)] + Neural network fast surrogate [A. Pavoen PhD Thesis TU Berlin 2020]
- Beam emission spectroscopy [S. Bannmann et al 2023 JINST 18 P10029]
- Langmuir probes [L. Rudischhauser et al. Rev. Sci. Instrum. 91, 063505 (2020)]
- 3D equilibrium magnetics [J. Schilling MSc Thesis Kiel University 2018] + Neural network fast surrogate [Andrea Merlo et al 2021 Nucl. Fusion 61 096039]
- Bolometry [J Svensson, S Kwak et al. to be published]
- Soft X-ray cameras [J. Schilling et al 2021 Plasma Phys. Control. Fusion 63 055010]
- Divertor spectroscopy [M. Krychowiak et al. EPS 2022]
- Heavy ion beam probes [H. Trimino Mora et al. HTPD 2024]
- Ellipsometry (stand-alone) [M. Krychowiak et al. HTPD 2024]

JET diagnostics

- Interferometers (Stand alone GPT application for profiles) [Svensson J. 2011 *EFDA–JET–PR(11)24* JET-EFDA]
- High-resolution TS system [Kwak S et al. 2020 *Nucl. Fusion* **60** 046009]
- Lithium beam diagnostics [Kwak S. et al. 2017 *Nucl. Fusion* **57** 036017] + Neural network fast surrogate [A Pavone et al 2020 PPCF 62 045019]
- ECE [S. Schmuck *et al* 2020 *Nucl. Fusion* **60** 066009]
- Polarimeters [Ford O. et al. 2008 *Rev. Sci. Instrum.* **79** 10F324]
- Magnetics (pickups, saddles, flux loops) [Svensson J. and Werner A. 2008 *Plasma Phys. Control. Fusion* **50** 085002]
- Current tomography [Svensson J. and Werner A. 2008 *Plasma Phys. Control. Fusion* **50** 085002]
- Equilibrium [Sehyun Kwak *et al* 2022 *Nucl. Fusion* **62** 126069]
- Z_{eff} profiles [Svensson J., JET Internal report]
- Divertor camera [Svensson J., JET Internal report]
- Soft X-ray [Li D. et al. 2013 *Rev. Sci. Instrum.* **84** 083506]

Optimal design for diagnostics (Interferometers, etc.)

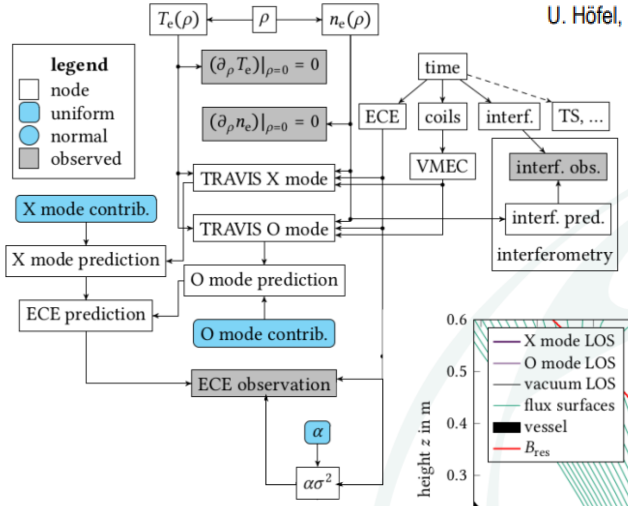
ITER diagnostics

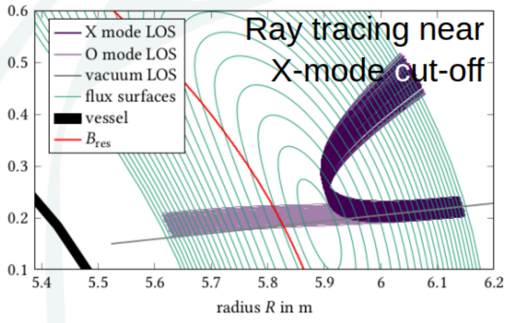
- Interferometers (TIP, DIP) [Deliverable 3, IO/20/CT/4300002304]
- Polarimeters (TIP, DIP, PoPola) [Deliverable 3, IO/20/CT/4300002304]
- ECE [Work in progress]
- Magnetics (pickups, flux loops, Rogowskis) [Deliverable 2, IO/20/CT/4300002304]
- X-ray crystal spectroscopy (core, edge, survey) [Deliverable 4, IO/20/CT/4300002304]
- Soft X-ray (radial) [Deliverable 4, IO/20/CT/4300002304]
- Hard X-ray (top, bottom) [Deliverable 4, IO/20/CT/4300002304]
- Visible spectroscopy (Z_{eff} bremsstrahlung, H-alpha, synchrotron, real-time Z_{eff} in PCS) [IO/21/CT/4300002467]

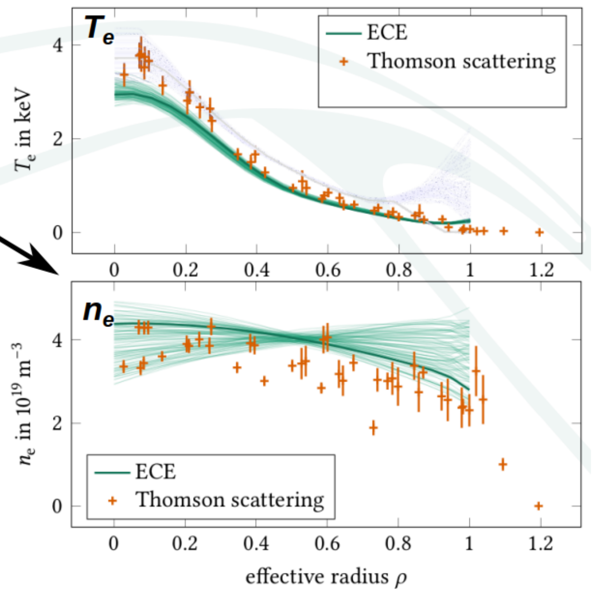
Minerva models and applications

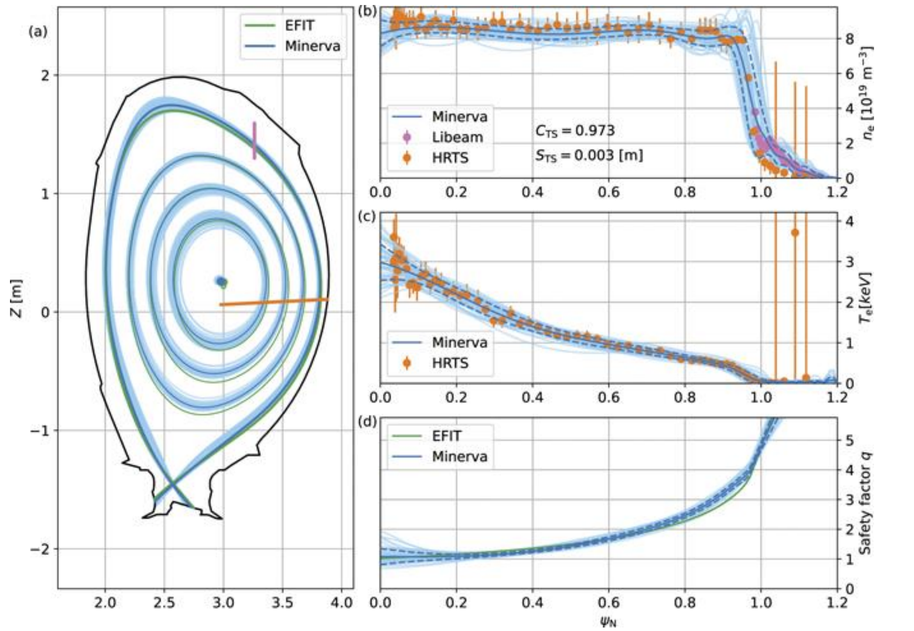
Sehyun Kwak *et al* 2022 *Nucl. Fusion* **62** 126069

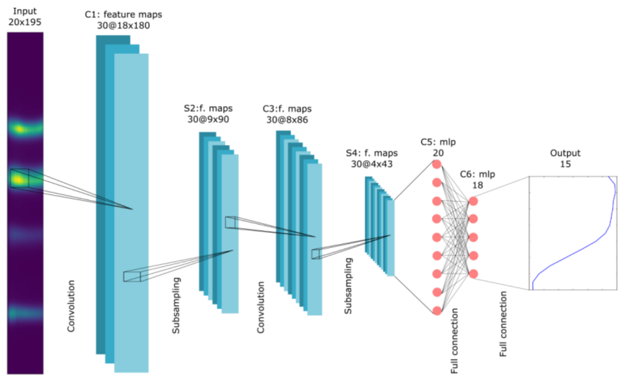
U. Höfel, „*Bayesian Analysis of Electron Cyclotron Emission Measurements at Wendelstein 7-X*" PhD thesis (2020)











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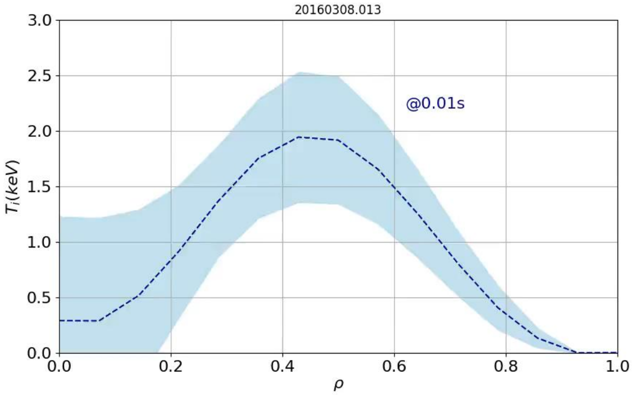
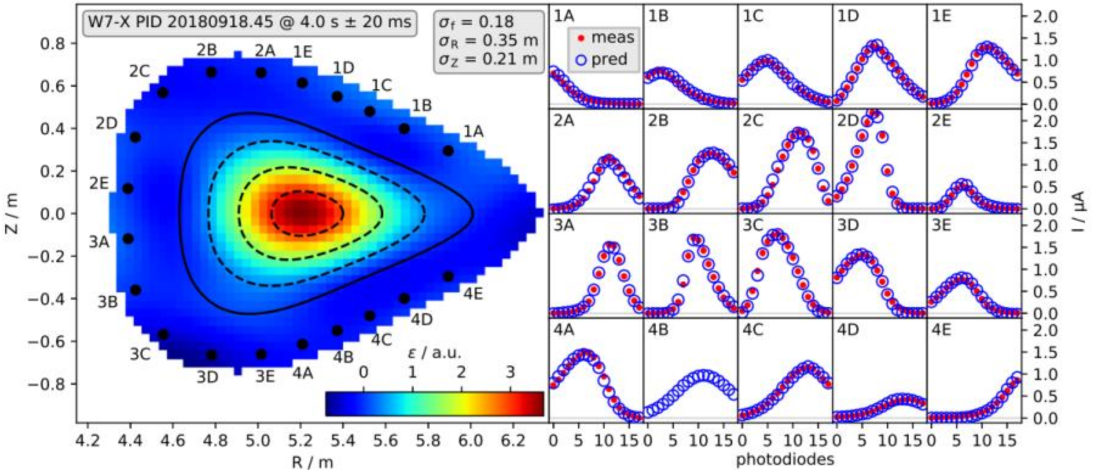
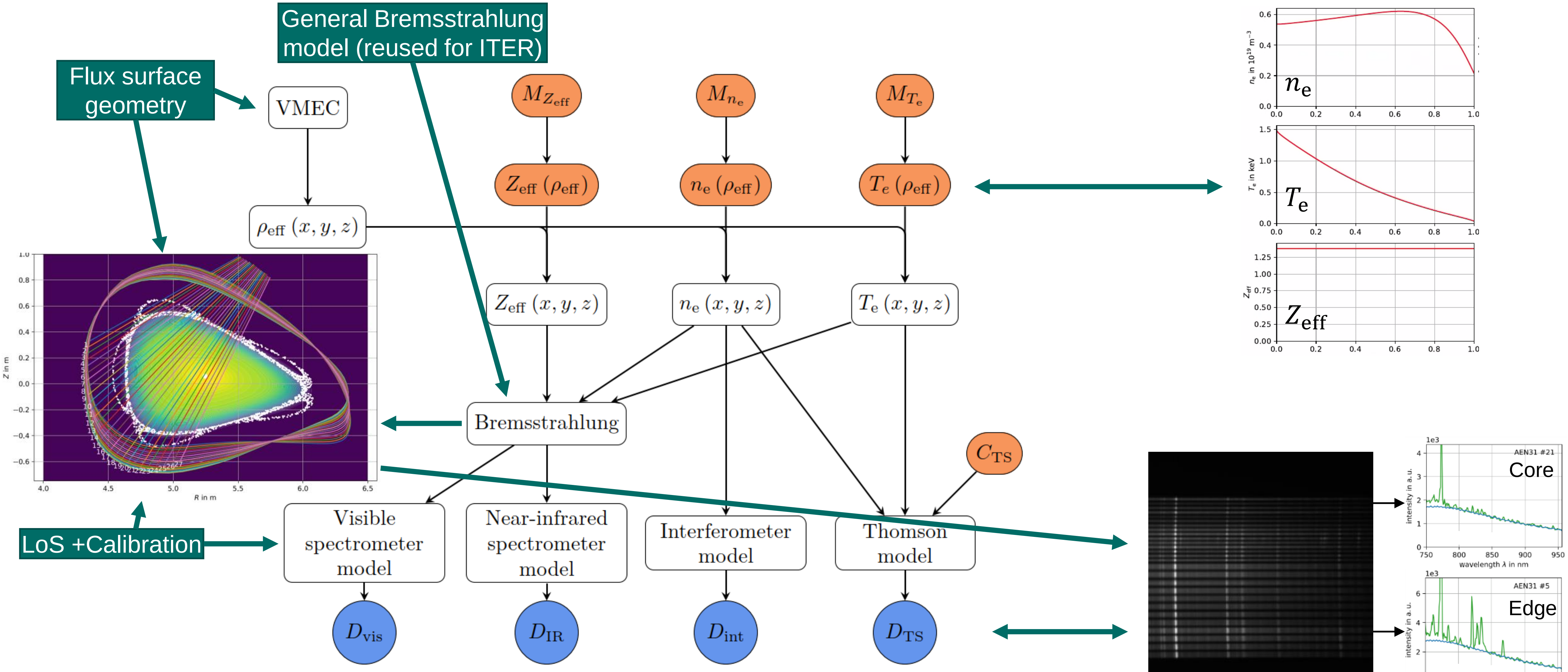




Jonathan Schilling *et al* 2021 *Plasma Phys. Control. Fusion* 63 055010

Application: Z_{eff} profiles from line integrated bremsstrahlung



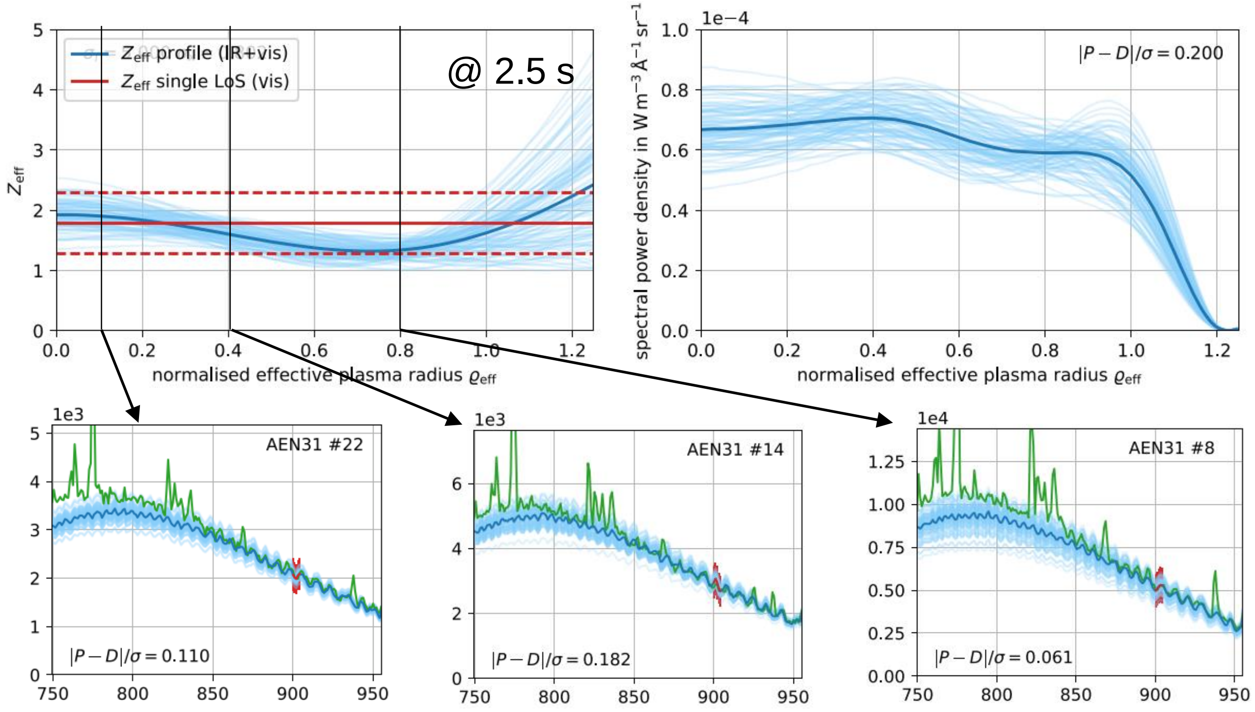
Inference solution:

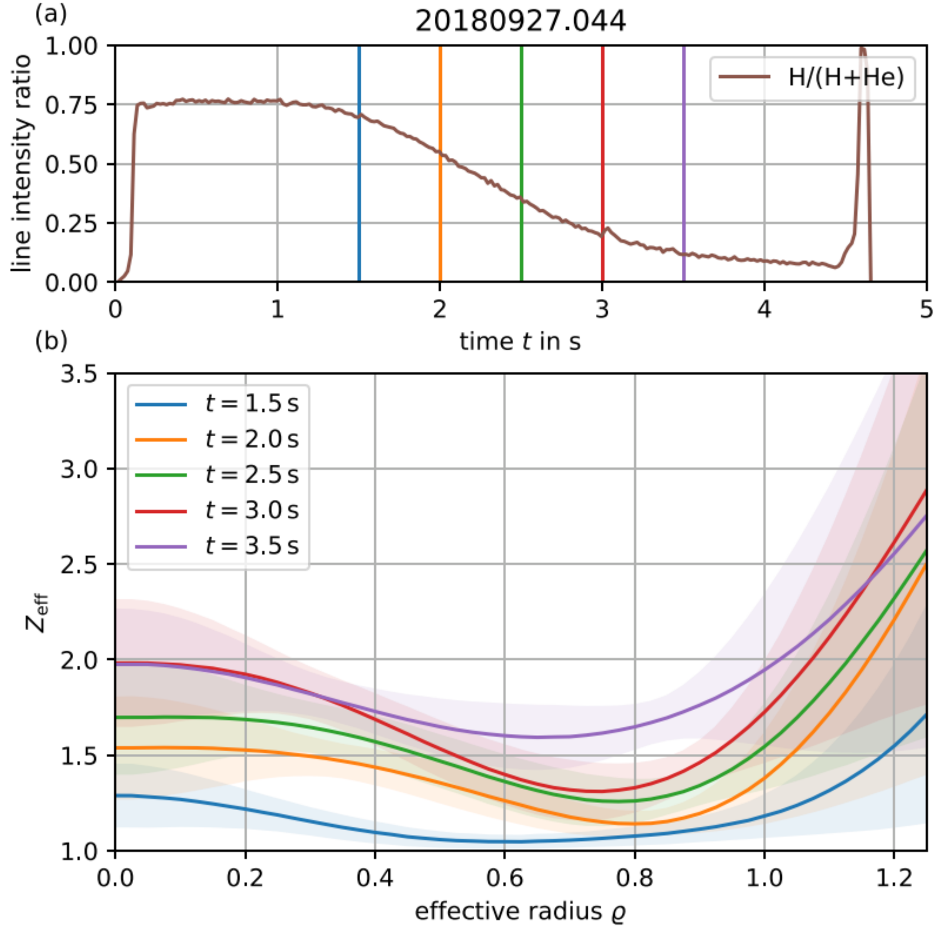
$$P(Z_{\mathrm{eff}}|D_{\mathrm{vis}}, D_{\mathrm{IR}}, n_e, T_e) \propto P(D_{\mathrm{vis}}, D_{\mathrm{IR}}|Z_{\mathrm{eff}}, n_e, T_e)P(Z_{\mathrm{eff}})$$

Kwak S. *et al.* 2021 *Rev. Sci. Instrum.* **92** 043505

Application: Z_{eff} profiles from line integrated bremsstrahlung

- Example discharge: H → He plasma
  - Increasing overall Z_{eff} over time
  - Well predicted line integrated bremsstrahlung spectra

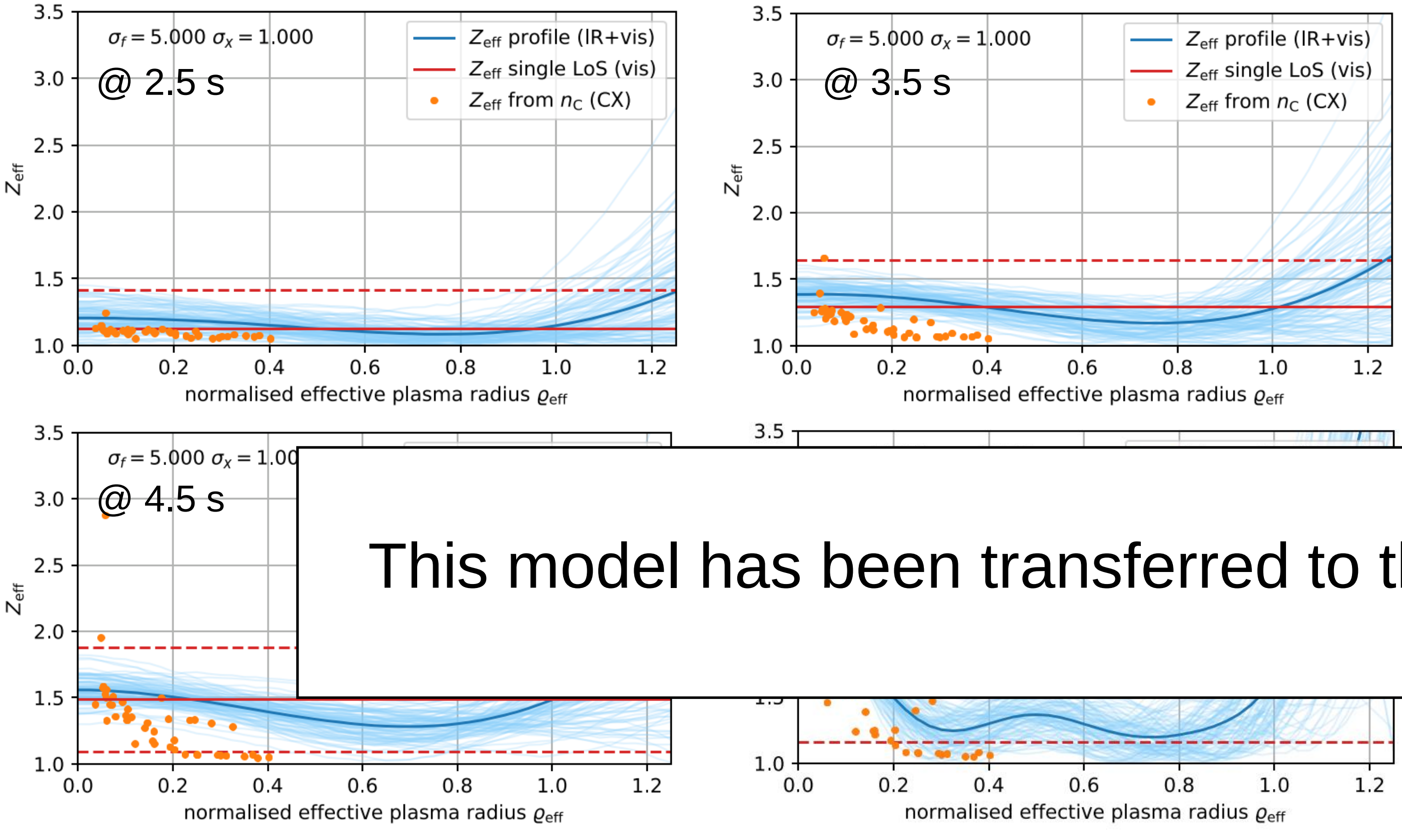


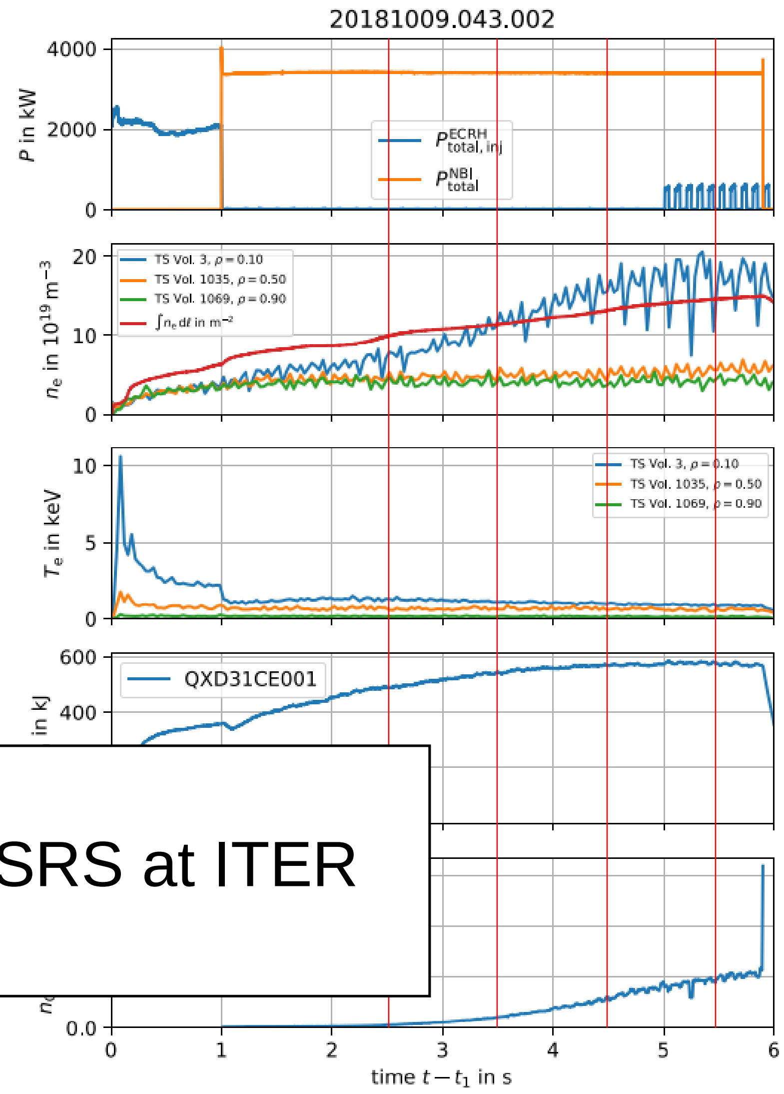


Kwak S. *et al.* 2021 *Rev. Sci. Instrum.* **92** 043505

Application: Z_{eff} profiles from line integrated bremsstrahlung

- Example discharge: Carbon accumulation
  - Consistent with estimated Z_{eff} values from CX spectrometers



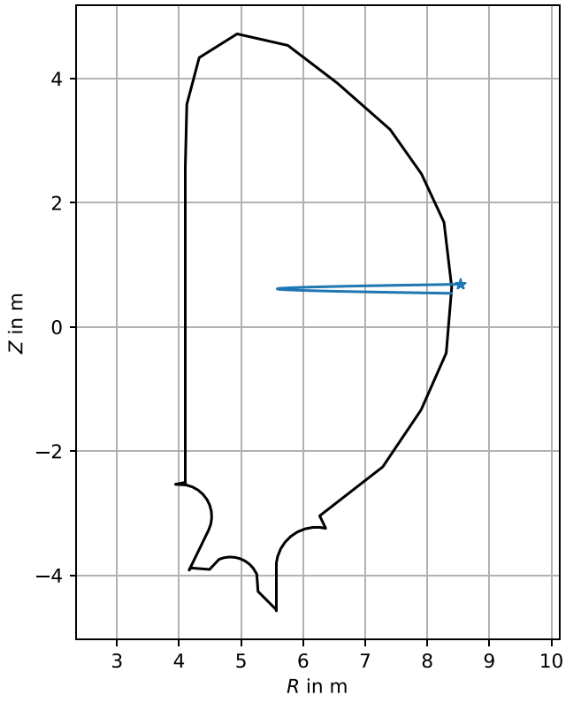


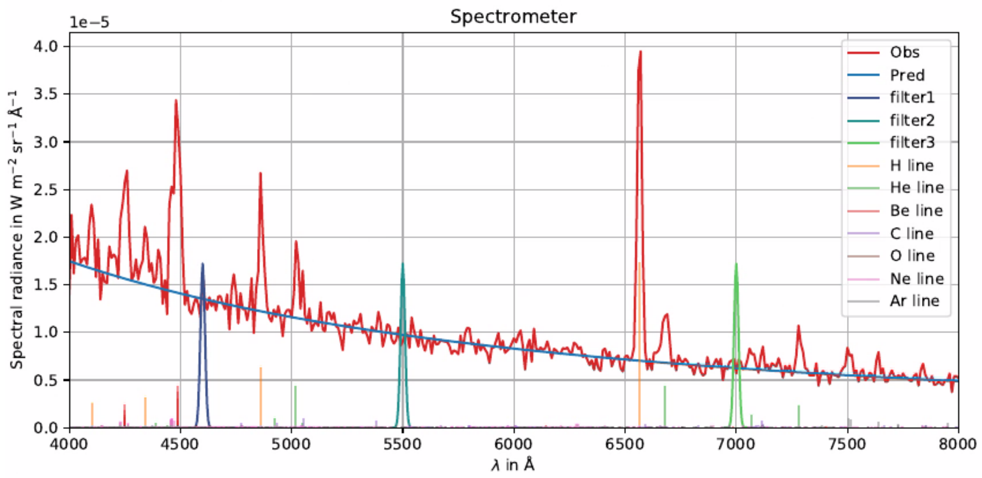
This model has been transferred to the VSRS at ITER

Kwak S. *et al.* 2021 *Rev. Sci. Instrum.* **92** 043505

Visible spectroscopy reference system at ITER

- The visible spectroscopy reference system (VSRS) collects the visible spectrum along a single line of sight through the plasma core to extract information on both the overall impurity content and the individual impurity species.
- The VSRS provides polychromator signals every 10 ms and a complete visible spectrum every 100 ms.
- The polychromator has three dedicated channels for measuring bremsstrahlung within interference filter windows approximately 4 to 6 nm wide, centred at 475.5, 547.5 and 734.5 nm.
- The full spectrum is used to obtain comprehensive information on line emissions and bremsstrahlung.





S Kwak *et al Bayesian modelling of visible spectroscopy reference system at ITER*, to be published

The model

Prior distribution:

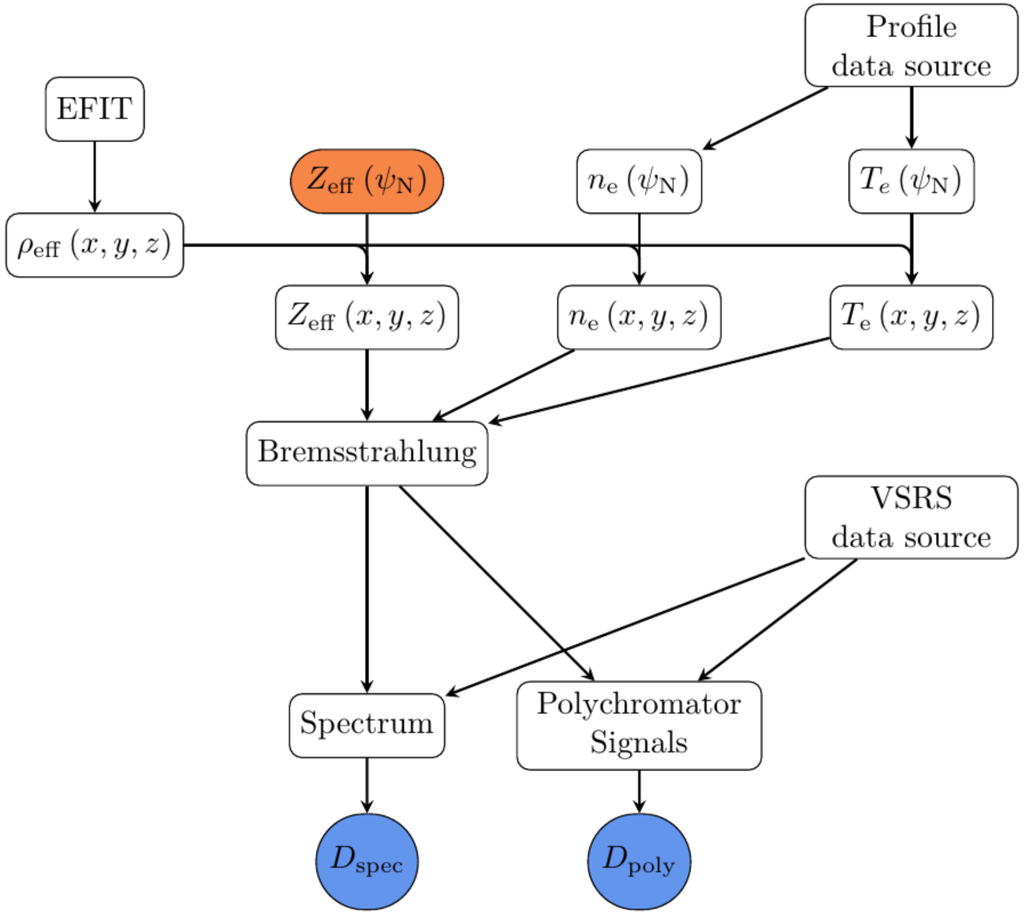
$$P(Z_{\text{eff}}) \sim U(1.0, 5.0)$$

Predictive distribution:

$$P\left(D_{\text{spec}}, D_{\text{poly}} \middle| Z_{\text{eff}}, n_{\text{e}}, T_{\text{e}}\right) \sim N(f(n_{\text{e}},\, T_{\text{e}},\, \psi_{\text{N}},\, Z_{\text{eff}}), \Sigma)$$

The inference solution:

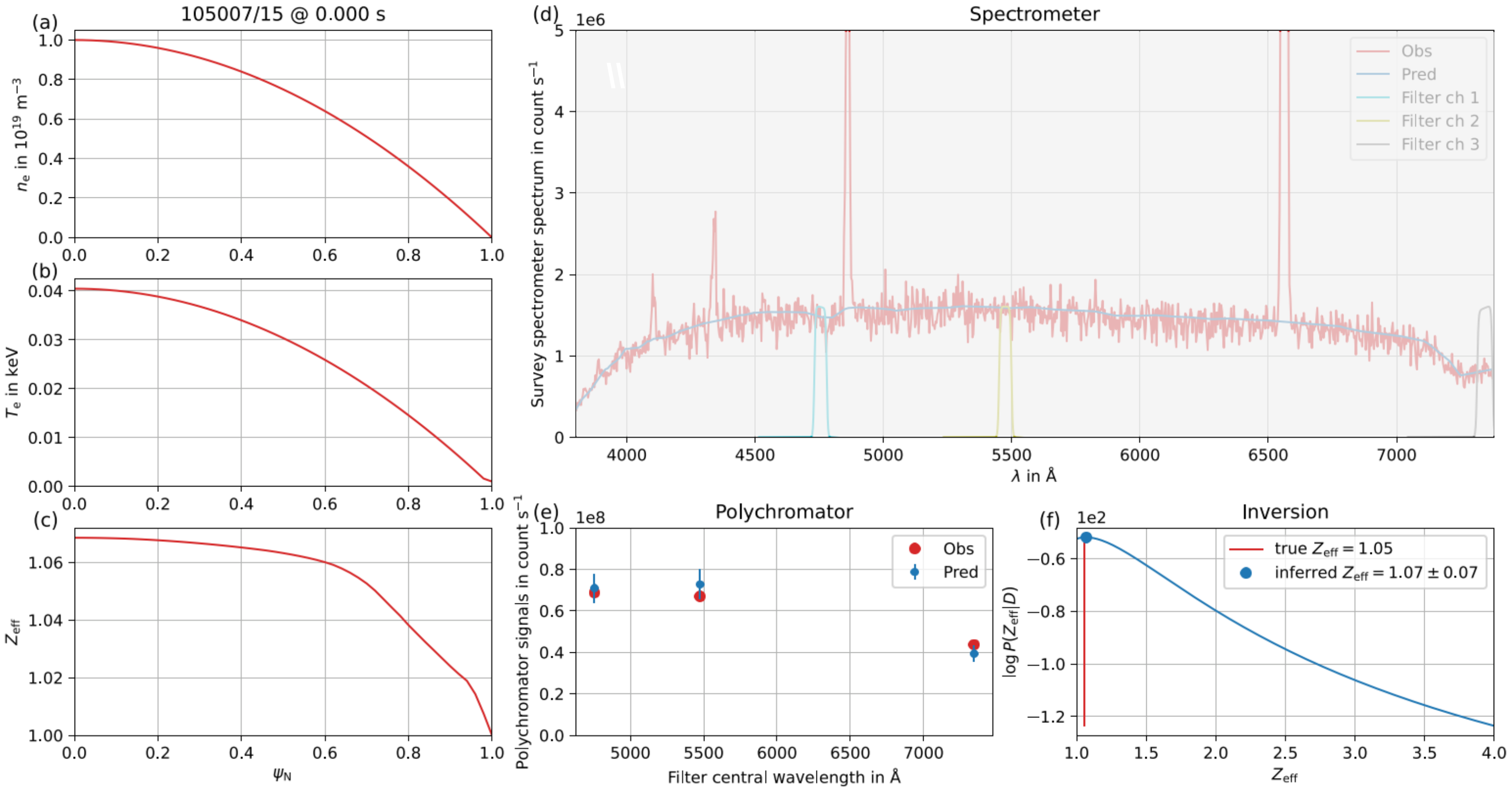
$$P\left(Z_{\text{eff}} \middle| D_{\text{spec}}, D_{\text{poly}}, n_{\text{e}}, T_{\text{e}}\right) \propto P\left(D_{\text{spec}}, D_{\text{poly}} \middle| Z_{\text{eff}}, n_{\text{e}}, T_{\text{e}}\right) P(Z_{\text{eff}})$$



S Kwak *et al Bayesian modelling of visible spectroscopy reference system at ITER*, to be published

Z_{eff} inference from spectrally integrated signals

- Synthetic data are generated for ITER scenarios and validated using the CASPER code.
- The MAP solution (blue dot) is closed to the underlying Z_{eff} value (red), given synthetic datasets
- Fast algorithm implemented for the ITER plasma control system

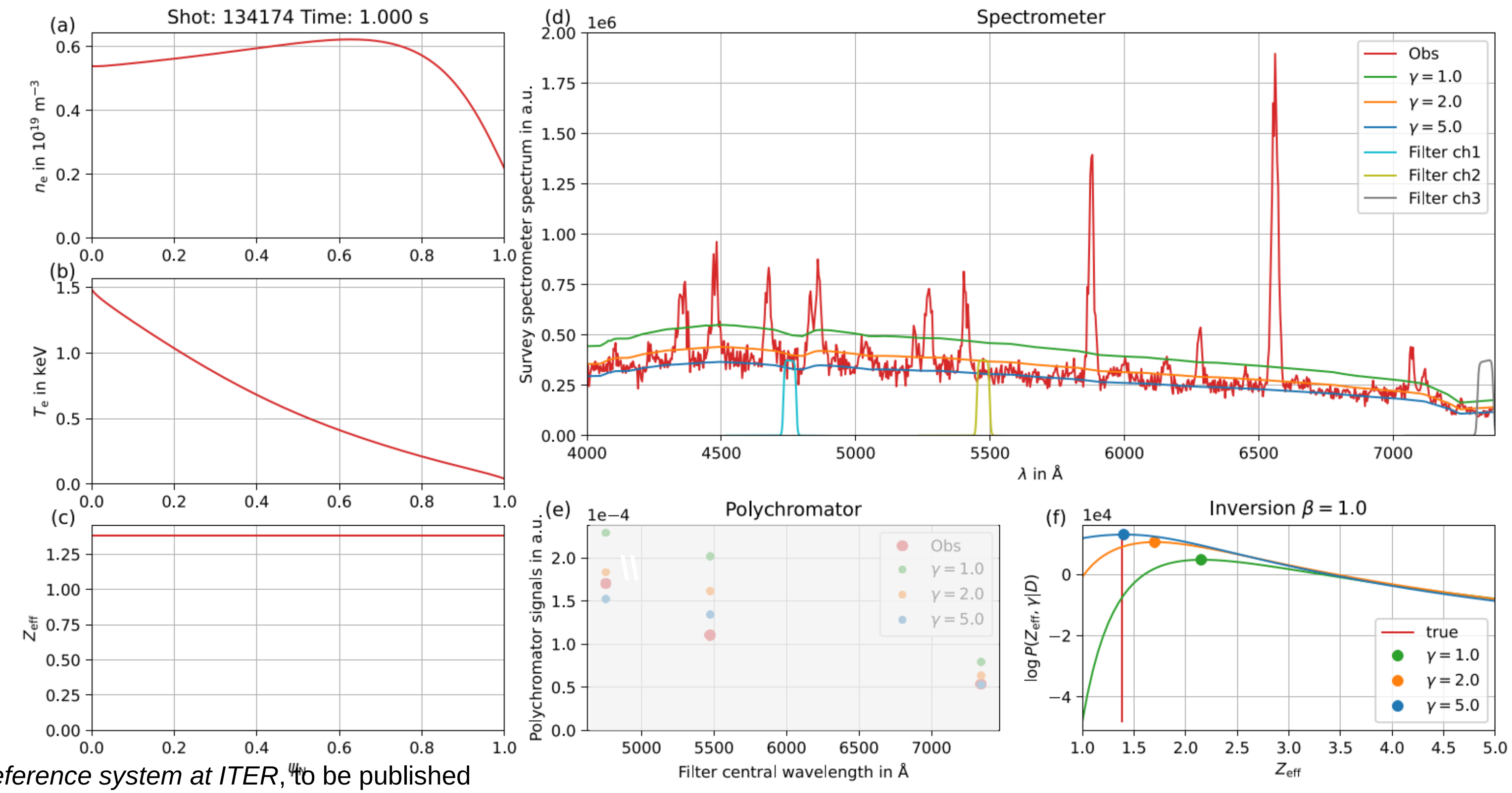


S Kwak *et al Bayesian modelling of visible spectroscopy reference system at ITER*, to be published

Z_{eff} inference from a full spectrum

- Spectral lines in the spectrum appear as outliers when inferring the background level.
- By applying an anomaly detection technique with asymmetric uncertainties, it is possible to automatically separate the spectral lines from the background continuum.

$$P(D_{\mathrm{spec},i}|Z_{\mathrm{eff}},\beta) = (1-\beta)\,P(D_{\mathrm{spec},i}\mid V_{\mathrm{spec},i},\sigma_i^2) + \beta\,P_{\mathrm{line}}(D_{\mathrm{spec},i}\mid V_{\mathrm{spec},i},\sigma_i^2,\gamma)$$



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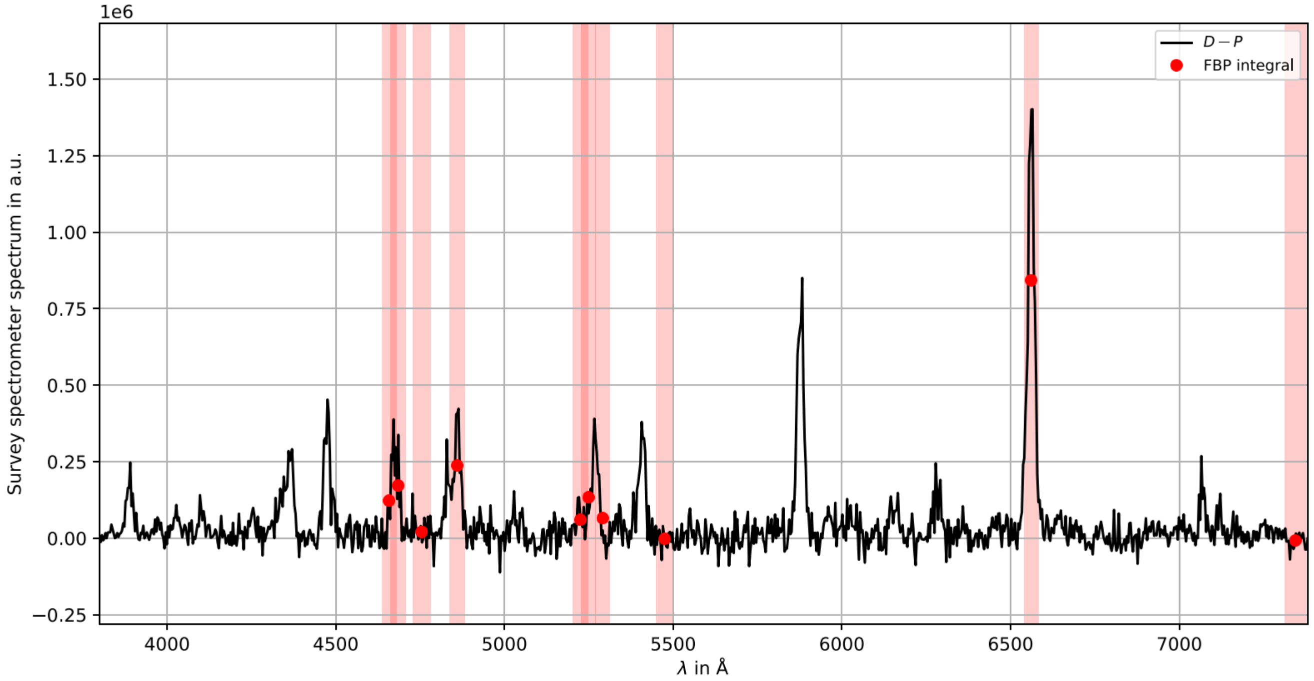
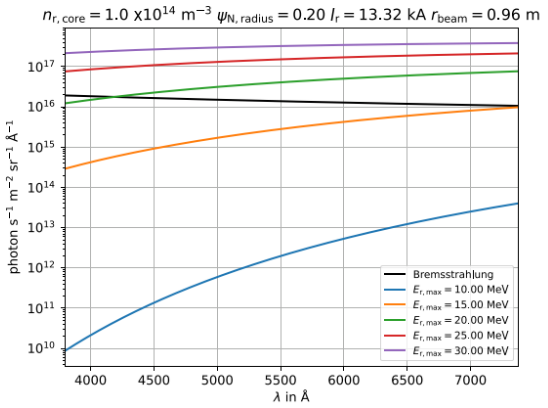
- Can also be used for automatic extraction of spectral lines.
- Can be applied to any spectra.

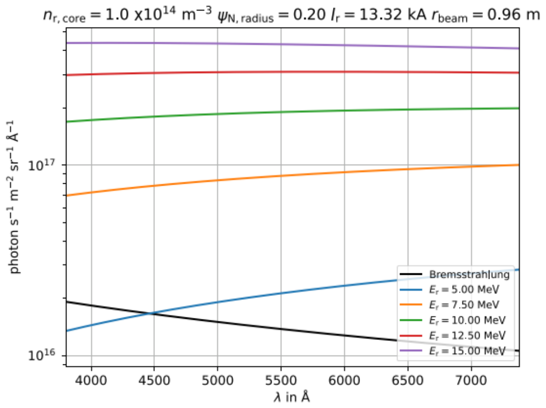


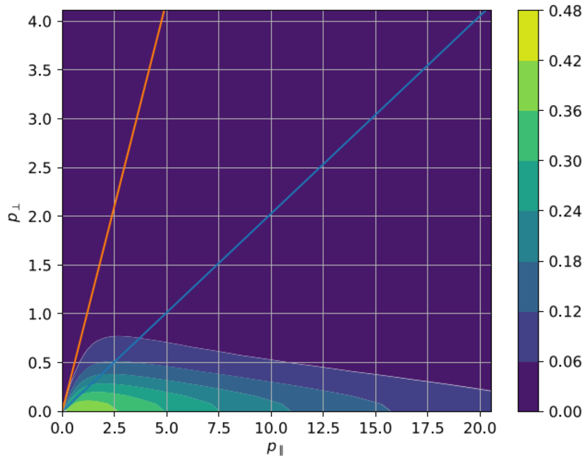
S Kwak *et al Bayesian modelling of visible spectroscopy reference system at ITER*, to be published

Summary

- Bayesian models for multiple plasma diagnostics have been developed for major fusion devices such as JET, W7-X, and ITER.
- The model, originally developed for Z_{eff} profile inference at W7-X, adapted for application to the ITER VSRS.
- A new method for the automatic separation of the background continuum has been developed and tested with synthetic data sets both with and without spectral lines.
- Based on the model, a fast algorithm for Z_{eff} inference has also been developed and will be implemented for real-time analysis at ITER.
- The feasibility of synchrotron detection with the VSRS was assessed using a physics-based forward model for synchrotron emission along the tangential line of sight.







Thank you for your attention!