

Integrated Data Analysis at ASDEX Upgrade

R. Fischer

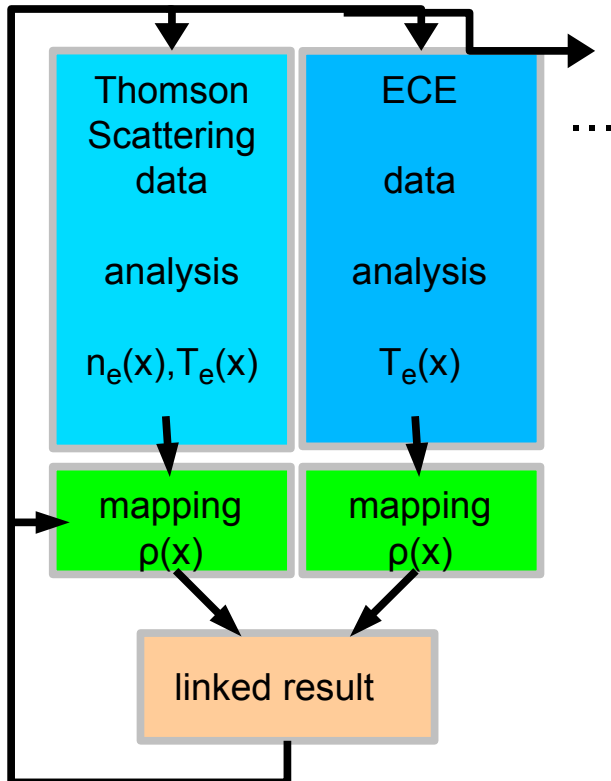
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ASDEX Upgrade, Garching, Jun 18, 2020

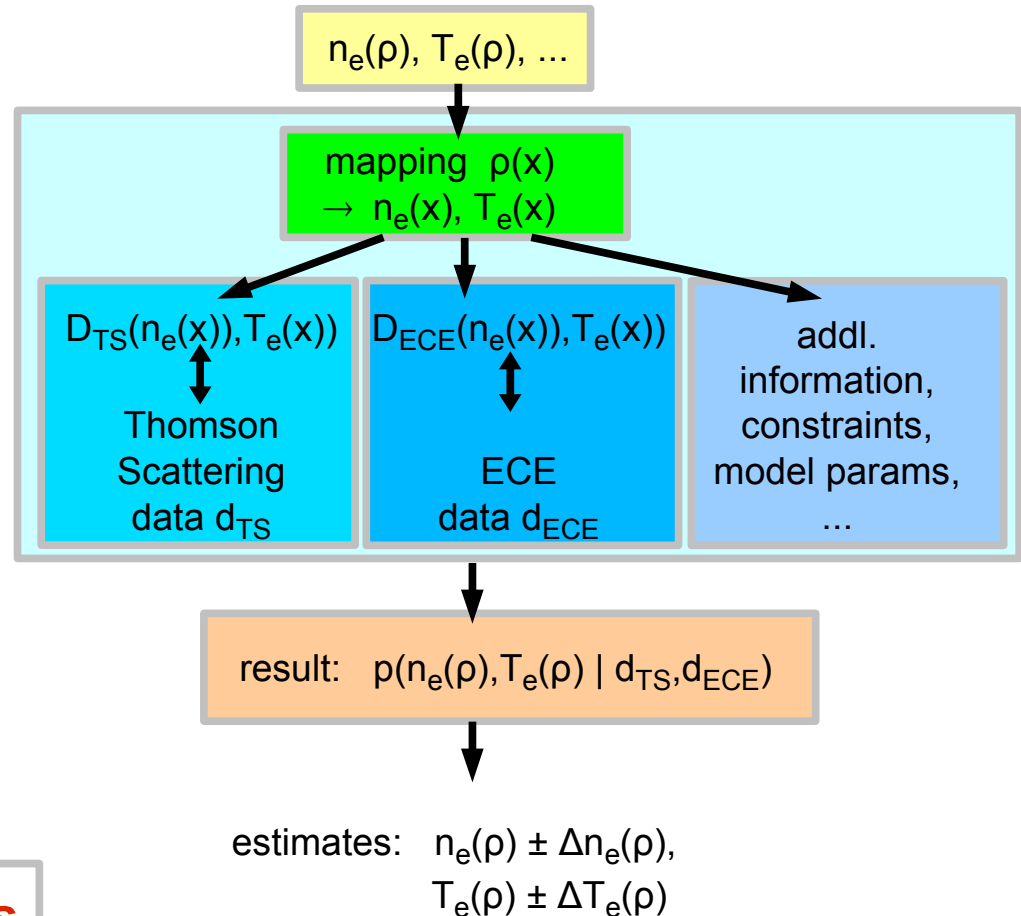
Conventional vs. Integrated Data Analysis



conventional



IDA (Bayesian probability theory)



Parametric entanglements

Drawbacks of conventional data analysis: iterative

- (self-)consistent results? (cumbersome; do they exist?)
- information propagation? (Single estimates as input for analysis of other diagnostics?)
- data and result validation? (How to deal with inconsistencies?)
- non-Gaussian error propagation? (frequently neglected: underestimation of the true error?)
- difficult to be automated (huge amount of data from steady state devices: W7X, ITER, ...)
- often backward inversion techniques (noise fitting? numerical stability? loss of information?)
- result: estimates and error bars (sufficient? non-linear dependencies?)

Probabilistic combination of different diagnostics (IDA)

- ✓ uses only forward modeling (complete set of parameters → modeling of measured data)
- ✓ additional physical information easily to be integrated
- ✓ systematic effects → nuisance parameters
- ✓ unified error interpretation → Bayesian Probability Theory
- ✓ result: probability distribution of parameters of interest

IDA offers a unified way
of combining data (information) from various experiments (sources)
to obtain improved results

Bayesian Recipe for IDA: LIB + DCN + ECE + TS



Reasoning about parameter n_e, T_e :

(uncertain) prior information

$$p(n_e, T_e)$$

prior distribution

+ experiment 1: $d_{LiB} = D_{LiB}(n_e, T_e) + \epsilon$; $p(d_{LiB} | n_e, T_e)$

+ experiment 2: $d_{DCN} = D_{DCN}(n_e) + \epsilon$; $p(d_{DCN} | n_e)$

+ experiment 3: $d_{ECE} = D_{ECE}(T_e) + \epsilon$; $p(d_{ECE} | T_e)$

+ experiment 4: $d_{TS} = D_{TS}(n_e, T_e) + \epsilon$; $p(d_{TS} | n_e, T_e)$

likelihood
distributions

+ *Bayes theorem*

$$p(n_e, T_e | d_{TS}, d_{ECE}, d_{LiB}, d_{DCN}) \propto p(d_{TS} | n_e, T_e) \times$$
$$p(d_{ECE} | T_e) \times$$
$$p(d_{LiB} | n_e, T_e) \times$$
$$p(d_{DCN} | n_e) \times$$
$$p(n_e, T_e)$$

posterior
distribution

+ additional uncertain (nuisance) parameter \rightarrow *marginalization*
generalization of Gaussian error propagation laws

Likelihood probability distribution



measured data: $d = D(T_e) + \epsilon$

modeled data: $D(T_e)$

noise (measurement uncertainty): ϵ

Likelihood: $p(d|T_e) = p(\epsilon = d - D(T_e))$

Example: Gaussian (independent, normally distributed measurement errors)

measurement uncertainty: $\sigma : p(\epsilon) \sim \exp\left(-\frac{\epsilon^2}{2\sigma^2}\right)$

$$p(\vec{d}|T_e, \vec{\sigma}) = \prod_i^N p(d_i|T_e, \sigma_i)$$
$$= \frac{1}{\prod_i^N \sqrt{2\pi\sigma_i^2}} \exp\left\{-\frac{\chi^2}{2}\right\} \quad \text{with} \quad \chi^2 = \sum_i^N \frac{[d_i - D_i(T_e)]^2}{\sigma_i^2}$$

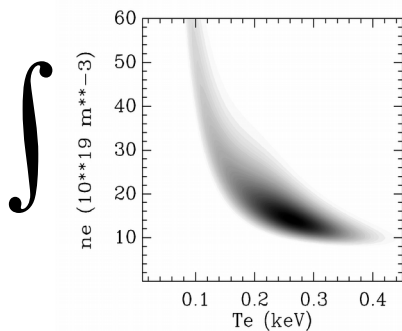
many variants: Poisson, Cauchy for outliers (robust estimation), ...

W7-AS:

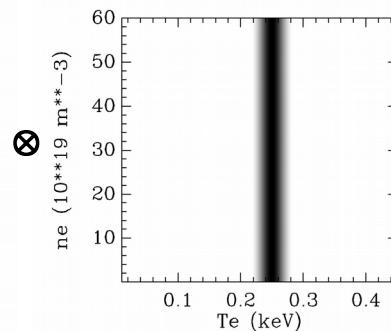
n_e, T_e : Thomson scattering, interferometry, soft X-ray

R. Fischer, A. Dinklage, and E. Pasch, Bayesian modelling of fusion diagnostics, Plasma Phys. Control. Fusion, 45, 1095-1111 (2003)

Using synergism: Combination a *set* of diagnostics

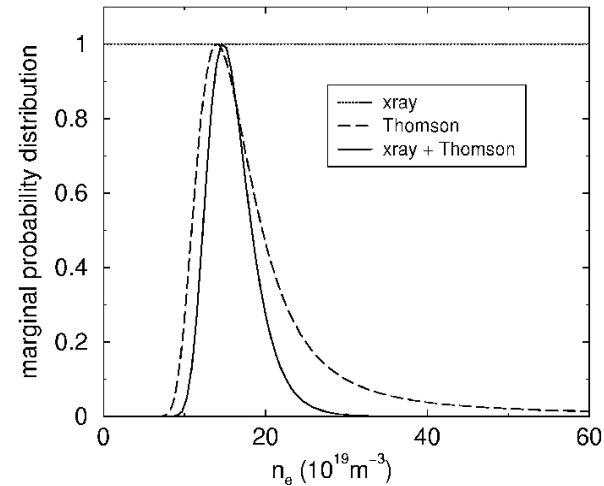


Thomson Scattering



Soft-X-ray

$$\otimes dT_e =$$



Electron density

30% reduced error

→ synergism by exploiting full probabilistic correlation structure

- *JET*: n_e , T_e : Interferometry, core LIDAR and edge LIDAR diagnostics
O Ford, et al., Bayesian Combined Analysis of JET LIDAR, Edge LIDAR and Interferometry Diagnostics, P-2.150, EPS 2009, Sofia
- *JET*: n_e Lithium beam forward modelling
D. Dodt, et al., Electron Density Profiles from the Probabilistic Analysis of the Lithium Beam at JET, P-2.148, EPS 2009, Sofia
- *TJ-II*: n_e Interferometry, reflectometry, Thomson scattering, and Helium beam
B. Ph. van Milligen, et al., Integrated data analysis at TJ-II: The density profile, Rev. Sci. Instrum. 82, 073503 (2011)
- *MST-RFP*: T_e from SXR and TS
L. M. Reusch, et al., An integrated data analysis tool for improving measurements on the MST RFP, Review of Scientific Instruments 85, 11D844 (2014)
- *W7-X*: $T_{e/i}$, n_e , impurity densities, flows, ... from X-ray imaging, TS, ...
e.g. A. Langenberg, et al., Inference of temperature and density profiles via forward modeling of an x-ray imaging crystal spectrometer within the Minerva Bayesian analysis framework, Review of Scientific Instruments 90(6), 063505 (2019)

and many more ...

(1) n_e, T_e : various profile diagnostics

R. Fischer et al., Integrated data analysis of profile diagnostics at ASDEX Upgrade, FST, 58, 675-684 (2010)

(2) T_i, v_{tor} :

- Gaussian process regression of various CXRS diagnostics

(3) Z_{eff} :

- Bremsstrahlung background from various CXRS diagnostic
- Impurity concentrations from CXRS

S. Rathgeber et al., Estimation of profiles of the effective ion charge at ASDEX Upgrade with Integrated Data Analysis, PPCF, 52, 095008 (2010)

(4) Improved equilibrium reconstructions: (→ next slides)

- Equilibrium code IDE
combining all measured data and
modeling information (current diffusion, fast-ion redistribution)

R. Fischer et al., FST (2016); R. Fischer et al., NF (2019)

Application: ASDEX Upgrade

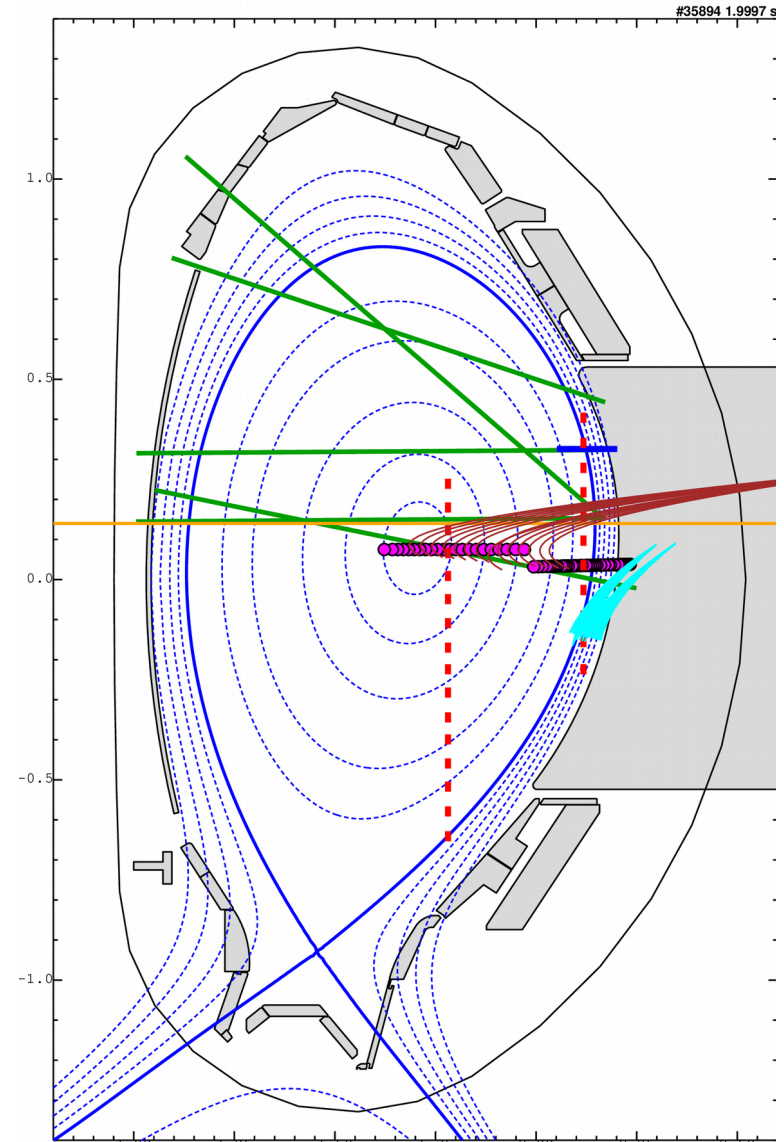


(1) *multi-diagnostic profile reconstruction: n_e , T_e*

- Lithium beam impact excitation spectroscopy (LIB)
- Interferometry measurements (DCN)
- Electron cyclotron emission (ECE)
- Thomson scattering (TS)
- Reflectometry (REF)
- Beam emission spectroscopy (BES)
- Thermal helium beam spectroscopy (HEB)

(2) Equilibrium reconstructions for diagnostics mapping: New and flexible equilibrium code IDE

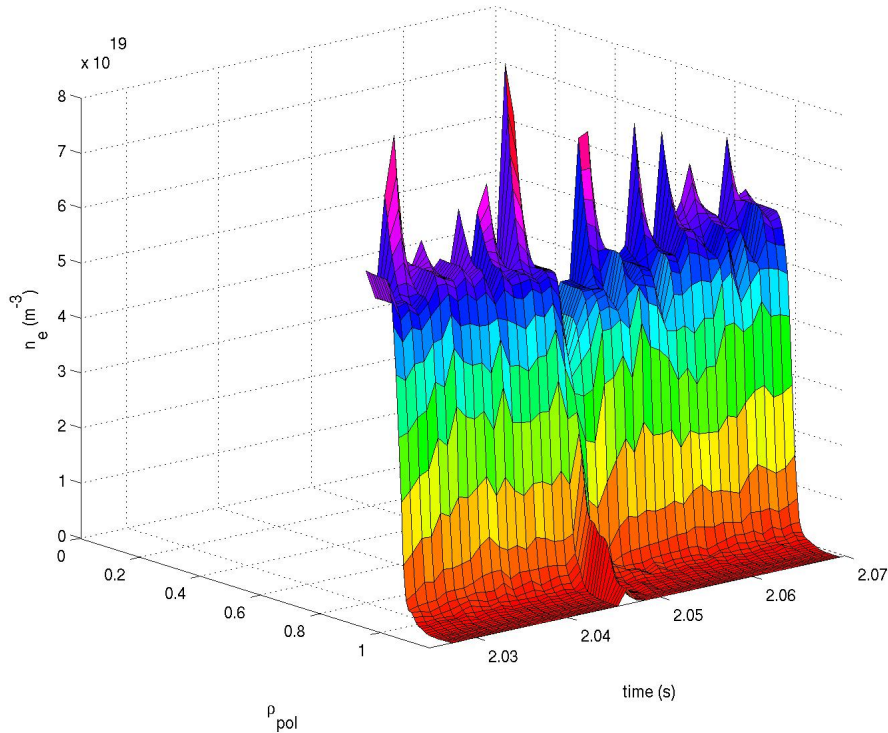
- Garching Parallel Equilibrium Code (GPEC)
- current diffusion
 - example: sawtooth reconnection



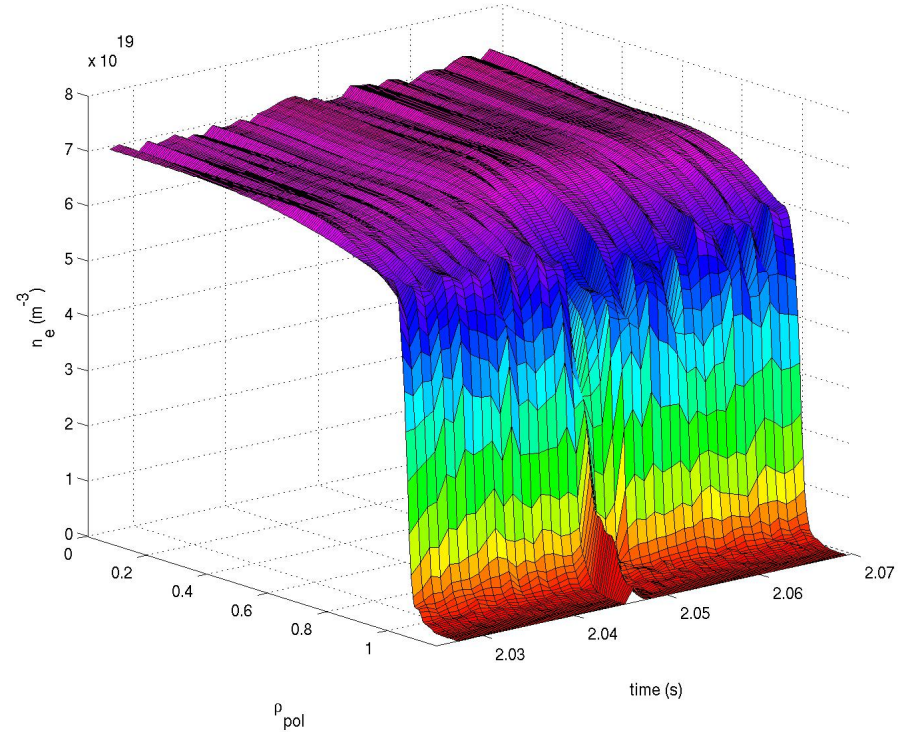
LIB + DCN: Temporal resolution



#22561, 2.045-2.048 s, H-mode, type I ELM



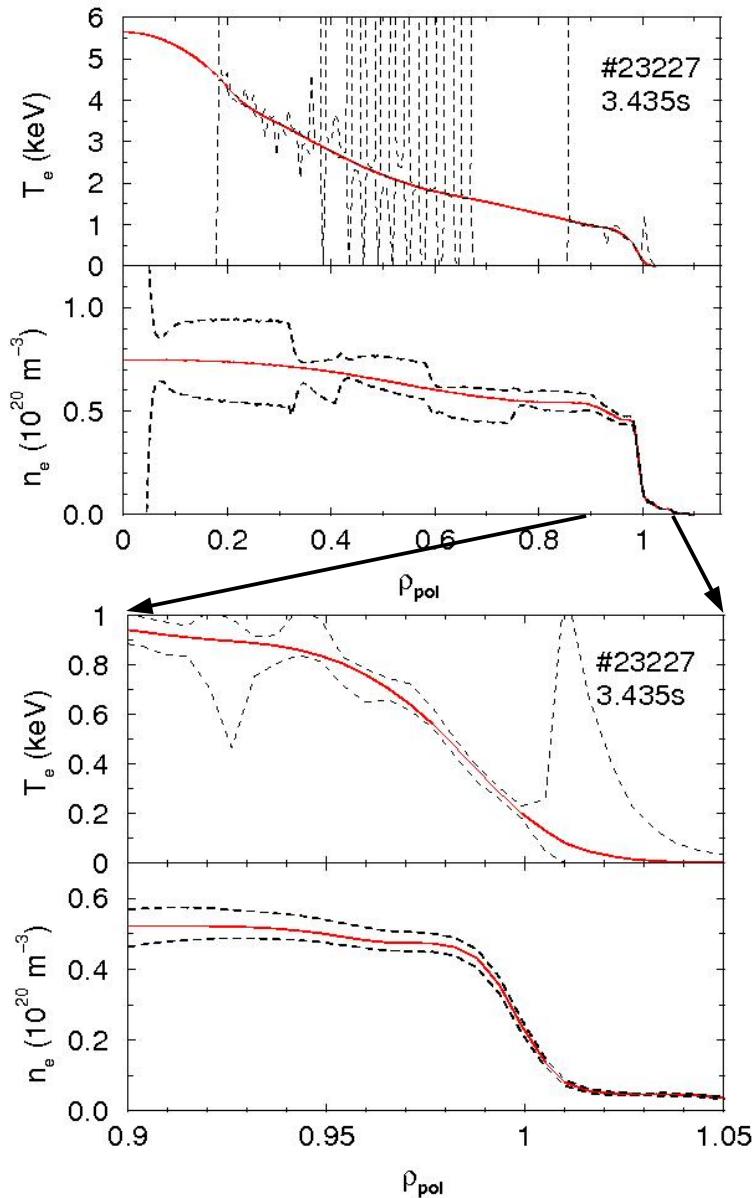
LIB: Lithium beam only



IDA: Lithium beam + DCN Interferometry

→ density profiles with high temporal resolution ($\geq 5 \mu\text{s}$)

IDA: LIB + DCN + ECE

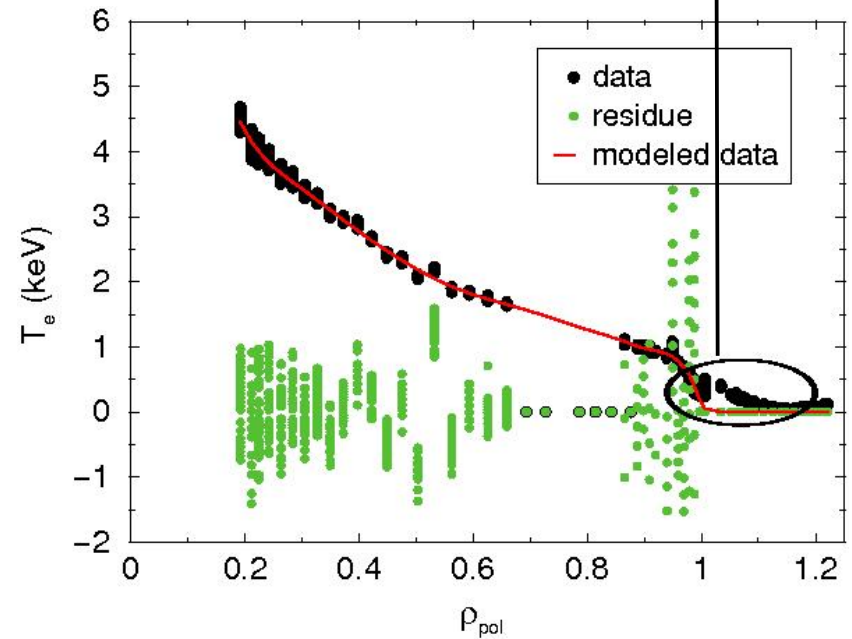


→ simultaneous:

- ✓ full density profiles
- ✓ (partly) temperature profiles

→ $n_e > 0.95 \cdot n_{e, \text{cut-off}}$ → masking of ECE channels

→ opt. depth $\sim n_e T_e$ → masking of ECE channels



IDA: LIB + DCN + ECE: radiation transport

- ECE assumptions: local emission and black-body radiation (optically thick plasma)

- Optically thin plasma (edge and core)

→ EC emission depends on T_e and n_e

→ combination with data from density diagnostics is mandatory

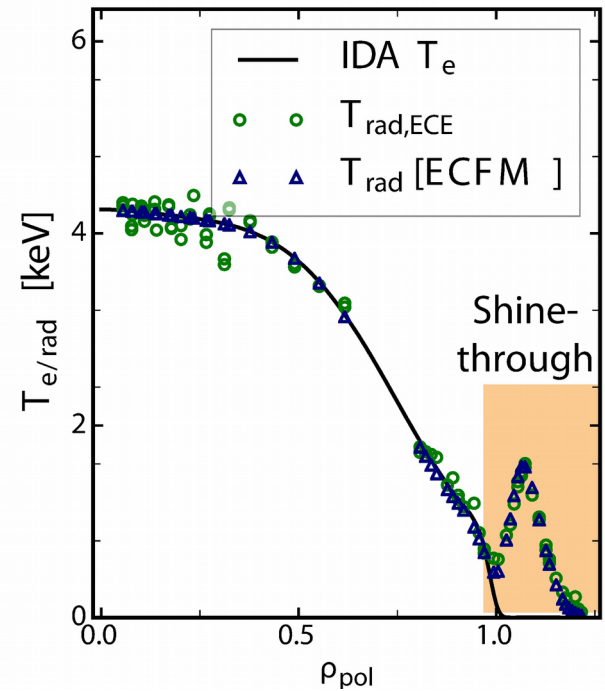
→ calculate broadened EC emission and absorption

profiles by solving the radiation transport equation

$$\frac{dI_\omega(s)}{ds} = j_\omega(s; n_e, T_e) - \alpha_\omega(s; n_e, T_e) I_\omega(s)$$

s LOS coordinate
 I_ω spectral intensity
 j_ω emissivity
 α_ω reabsorption

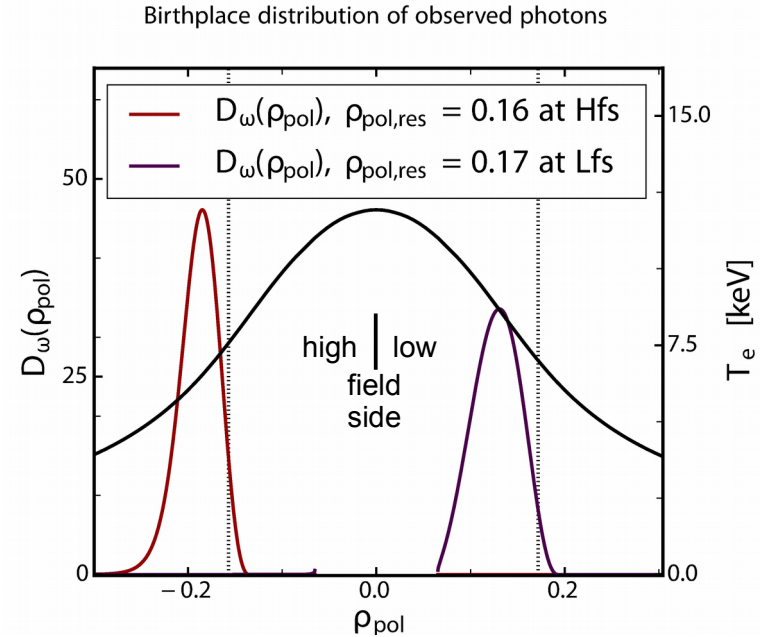
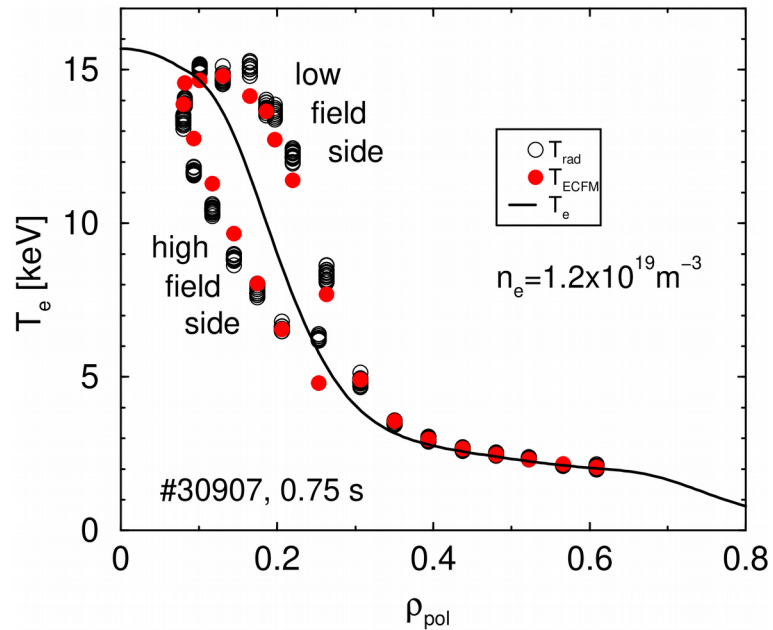
T_{Rad}, T_e for #30589 $t = 1.27$ s



- electron cyclotron forward model (ECFM) in the framework of Integrated Data Analysis

(S.K. Rathgeber et al., PPCF 55 (2013) 025004; S.S. Denk et al., PPCF 60 (2018) 105010)

ECE: Core shine-through



ECE core hfs-lfs loop if small optical depth in core (small n_e) and large core T_e -gradient:

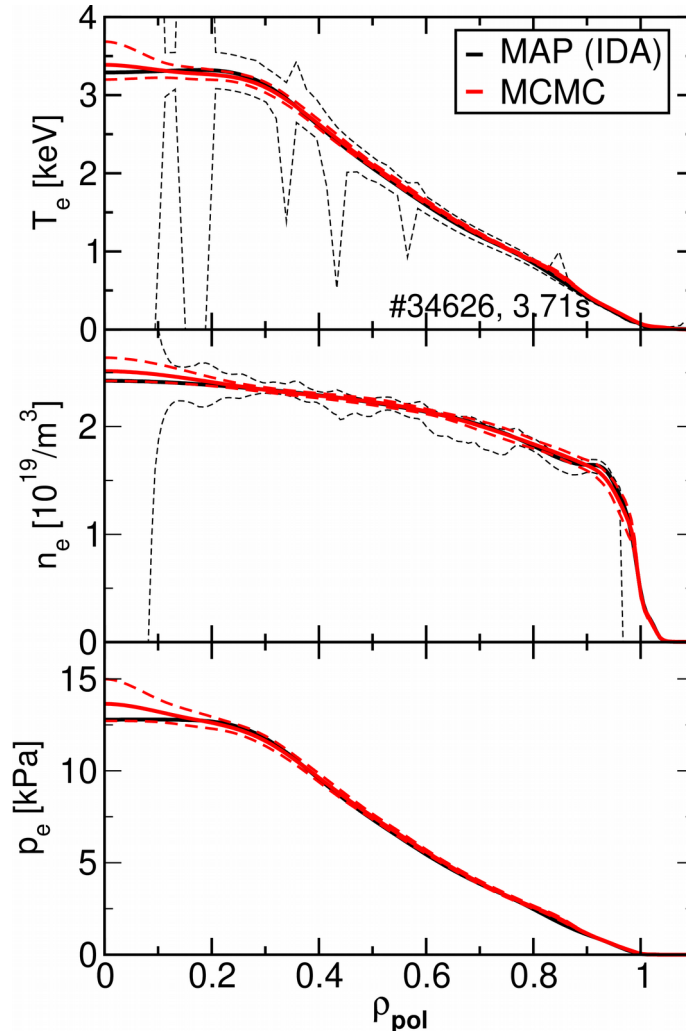
→ extended microwave emission region

→ high-field side: $T_{\text{rad}} < T_e$ due to shine-through of smaller (outer) temperatures

→ low-field side: $T_{\text{rad}} > T_e$ due to shine-through of larger (inner) temperatures

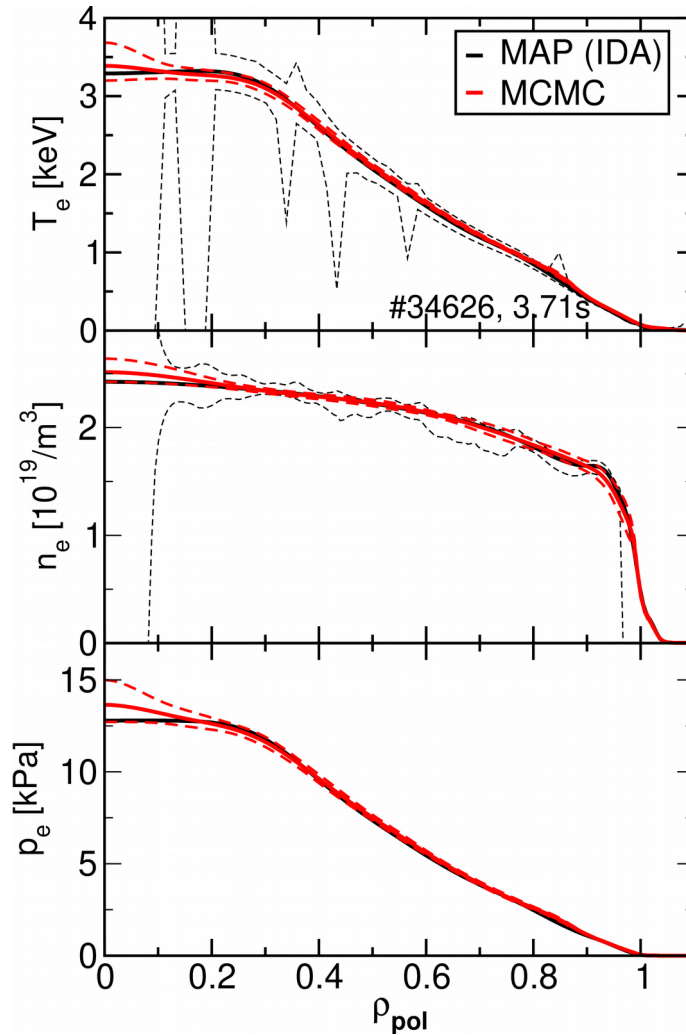
[“Non-thermal electron distributions measured with ECE”, S. Denk, Master thesis, 2014]

T_e , n_e , p_e profiles and uncertainties: MAP, MCMC

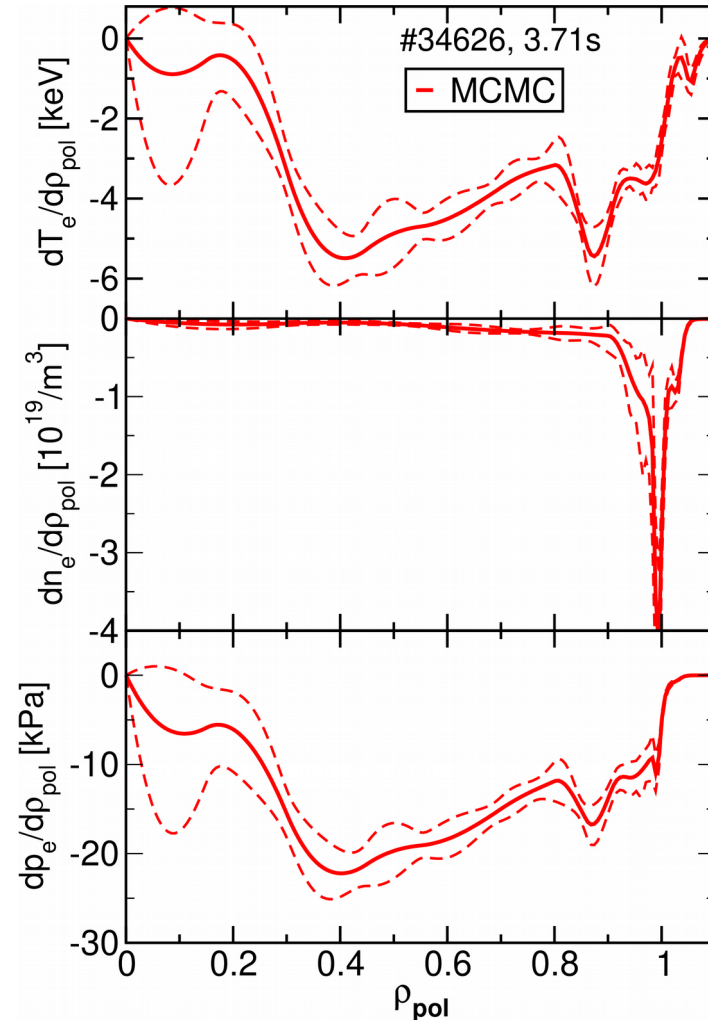


- Maximum a Posterior (MAP)
 - (T_e, n_e) estimate → IDA
 - error bar from lokal profile changes and effect on χ^2 (Fischer, PPCF 2008); without profile correlations
 - Markov chain Monte Carlo (MCMC) sampling of posterior probability distribution
 - mean → (T_e, n_e) estimate
 - variance → (small) error bar (incl. correlations)
 - profile samples
 - error propagation in modeling codes
- ! drawback: time consuming due to collisional radiative model for LIB radiation transport modeling for ECE
→ $\sim h / \text{time point}$

T_e , n_e , p_e gradients and uncertainties: MCMC

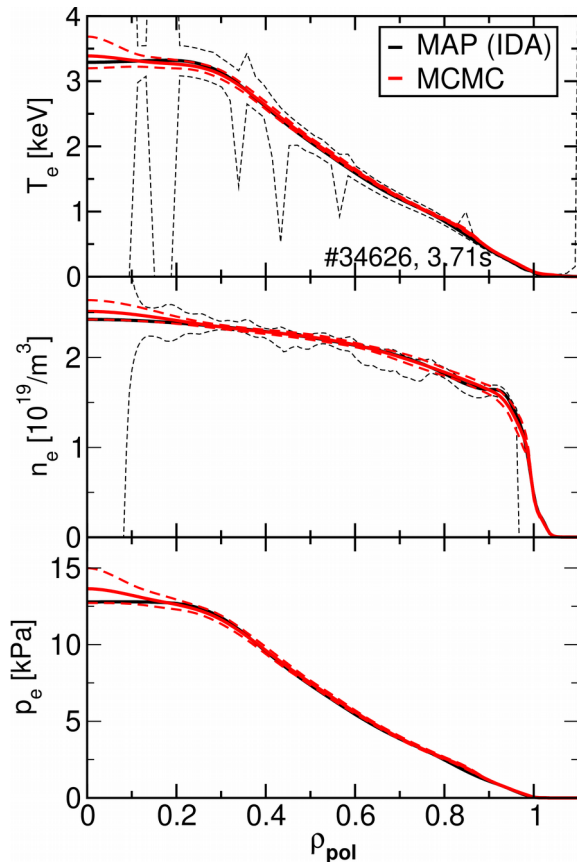


profiles

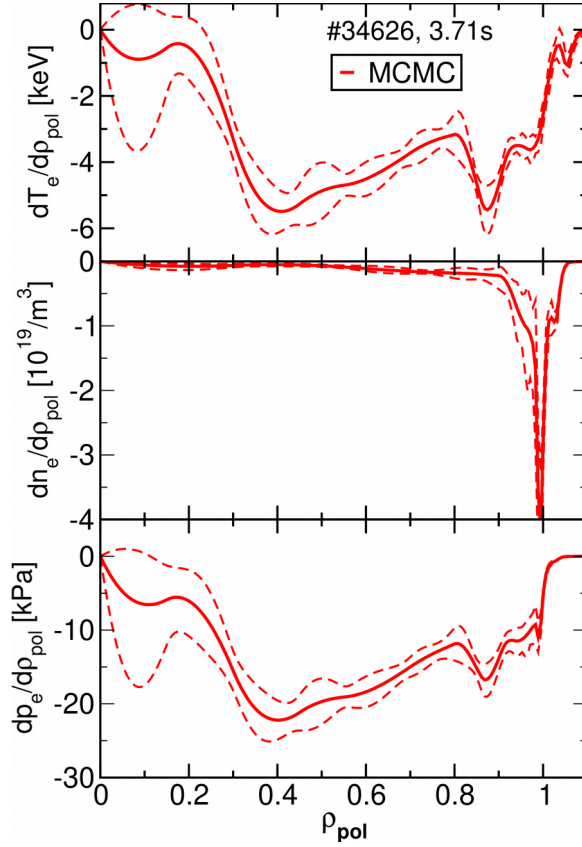


profiles gradients

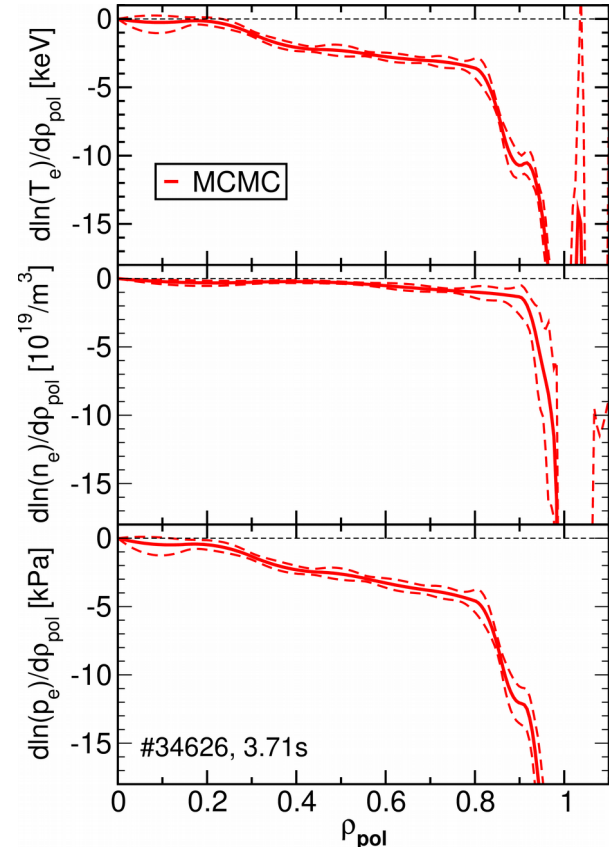
T_e, n_e, p_e logarithmic gradients and uncertainties



profiles



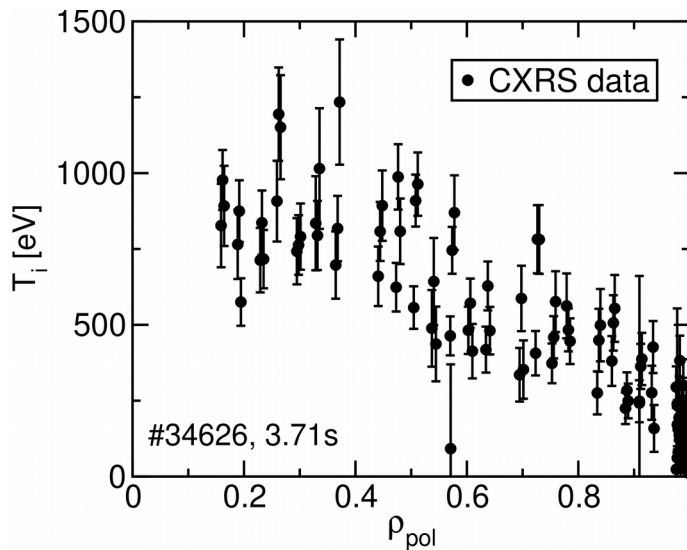
profile gradients



logarithmic profile gradients

→ GENE: UQ and UP (F. Jenko, C. Michoski, Univ. Texas Austin)

T_i : Gaussian process regression



- interpolation and smoothing of noisy data
- extrapolation to axis
- uncertainties of profiles and profile gradients

R.M. McDermott, RSI 2017

- Gaussian process (GP): random variable has (multidimensional) normal distribution
- GP regression (GPR):

→ no assumption about profile shape!

→ different positions are correlated depending on distance

→ likelihood

$$p(\vec{d}|f(x), \vec{\sigma}) = N(\vec{d}|f(x), \vec{\sigma})$$

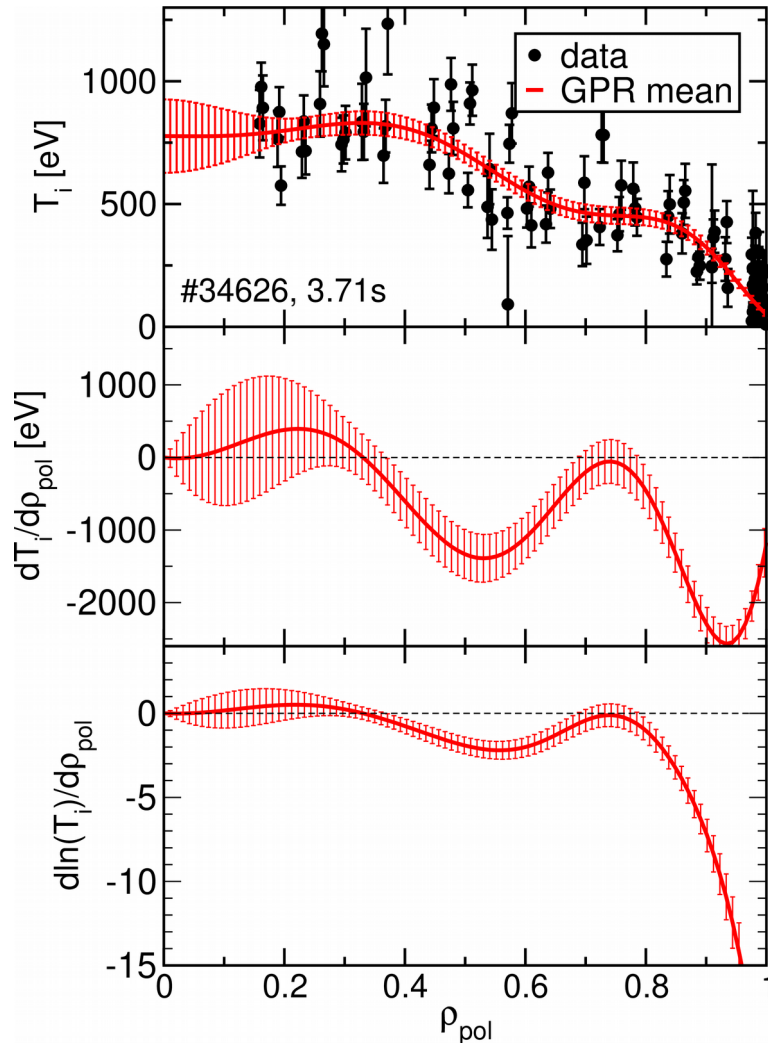
$$\text{Cov}(f_k, f_l) = \eta^2 \exp\left(-\frac{(x_k - x_l)^2}{2\xi^2}\right)$$

- Result: (Gaussian) probability distribution of possible interpolating functions

→ Mean/variance of pdf: Analytic solution for profile, gradients and their uncertainties

→ Samples of pdf: candidate profiles to study UP in modeling codes

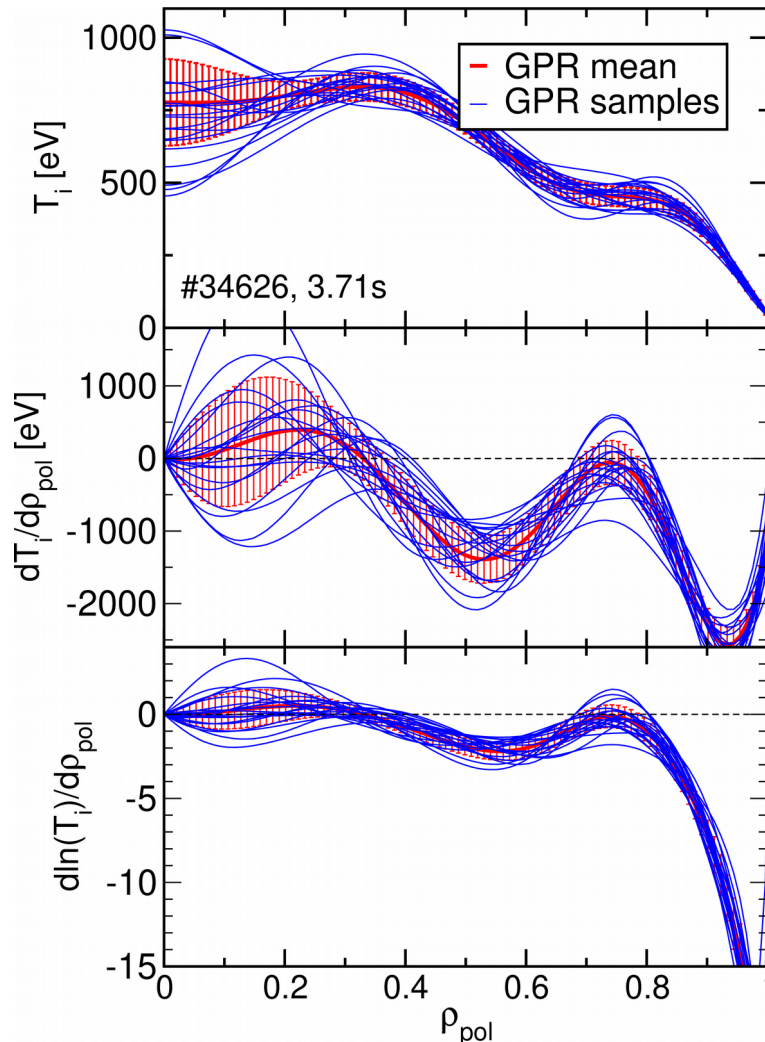
T_i : Profile, gradient and uncertainty



- estimation and uncertainty (1 std) of
 - T_i profile
 - T_i profile gradient
 - T_i profile logarithmic gradient
- result depends on parameters:
 - correlation length ξ
 - kernel weight η
- correlation length ξ :
 - might depend on position ρ_{pol} (*non-stationary*)
 - here: $\xi=0.25$ (core) → 0.20 (edge)
 - $\xi \downarrow \rightarrow$ uncertainty \uparrow
- constraint $dT_i/d\rho_{pol}=0$ at magn. axis

→ GENE: UQ and UP (F. Jenko, C. Michoski)

T_i : Samples of profiles and gradients

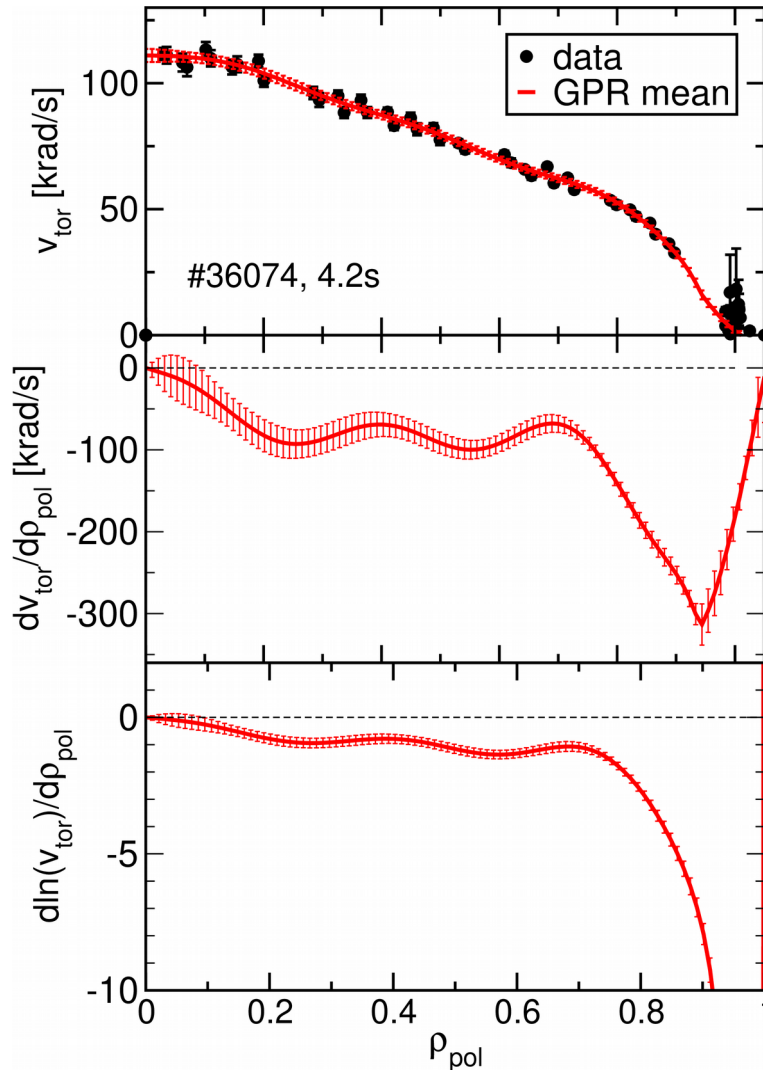


- samples of
 - T_i profile,
 - T_i profile gradient and
 - T_i profile logarithmic gradient

useful for uncertainty propagation (UP)
in modeling codes

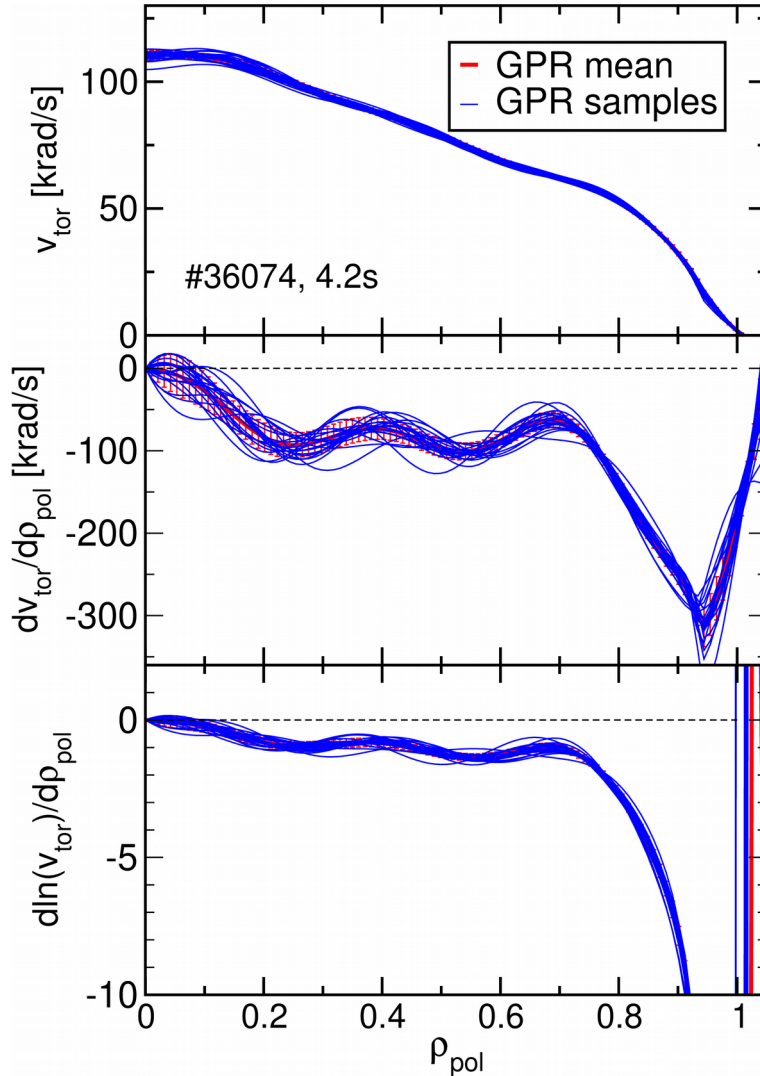
- mean and uncertainty of profiles, gradients, logarithmic gradients and covariance matrices for sampling
 - fast: ~ 6 s / 1000 time points
 - ASDEX Upgrade shotfile IDI

v_{tor} : Profile, gradient and uncertainty



- estimation and uncertainty (1 std) of
 - v_{tor} profile
 - v_{tor} profile gradient
 - v_{tor} profile logarithmic gradient
- constraint $dv_{\text{tor}}/d\rho_{\text{pol}}=0$ at magn. axis
- further applications: n_{imp}

v_{tor} : Samples of profiles and gradients



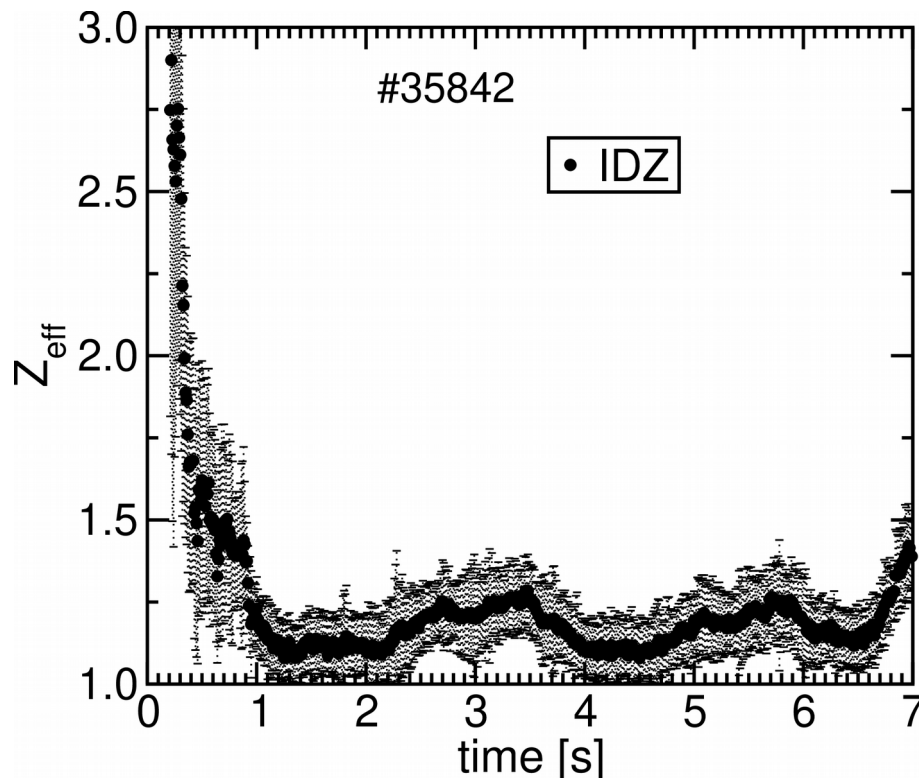
- samples of
 - v_{tor} profile,
 - v_{tor} profile gradient and
 - v_{tor} profile logarithmic gradient

useful for uncertainty propagation (UP)
in modeling codes

Z_{eff} estimate and uncertainty



- Z_{eff} : bremsstrahlung background of CXRS spectra (CER, COR, CUR, CAR, ...)
(Rathgeber, PPCF 2013)
- recently extended and validated (A. Kappatou, R.M. McDermott, F. Atour, Bachelor Thesis 2018)
- selection of core LOS without signal from reflections
- assume spatially constant Z_{eff} (Z_{eff} profile t.b.d.)



- uncertainty ~20%
- ASDEX Upgrade shotfile IDZ

Magnetic Equilibrium

The IDE equilibrium solver reconstructs the current distribution by solving the

1. **Grad-Shafranov equation:** Ideal magnetohydrodynamic equilibrium for poloidal flux function Ψ for axisymmetric geometry

$$\left(R \frac{\partial}{\partial R} \frac{1}{R} \frac{\partial}{\partial R} + \frac{\partial^2}{\partial z^2} \right) \Psi = -(2\pi)^2 \mu_0 (R^2 P' + \mu_0 F F')$$

subject to all available measured data (magnetics, pressure profile, polarimetry, (i)MSE, ... many more)
and (unphysical) smoothness constraints to regularize the ill-conditioned solver

coupled with the

2. **Current diffusion equation:** describes the diffusion of the poloidal flux Ψ on the background of the toroidal flux $\Phi(\rho)$ due to resistivity

$$\sigma_{\parallel} \frac{\partial \Psi}{\partial t} = \frac{R_0 J^2}{\mu_0 \rho} \frac{\partial}{\partial \rho} \left(\frac{G_2}{J} \frac{\partial \Psi}{\partial \rho} \right) - \frac{V'}{2\pi\rho} (j_{bs} + j_{ec} + j_{nb})$$

Goal: replace non-physical smoothness constraints

by a temporal correlation defined by the current diffusion

(→ ASDEX Upgrade shotfiles IDE, IDG, IDF)

Sawtooth crash: Current redistribution

Most important ingredients for sawtooth crash current estimation:

1. GSE:

- + pressure profiles: $p_e + p_i + p_{fast}$
- (+ polarimetry)
- (+ MSE and iMSE)

2. CDE (neoclassical current diffusion):

- + kinetic profiles (\rightarrow conductivity $\rightarrow T_e$):

$$T_e, n_e$$

$$T_i$$

$$n_i \sim f(n_e - n_{fast}); Z_{eff}$$

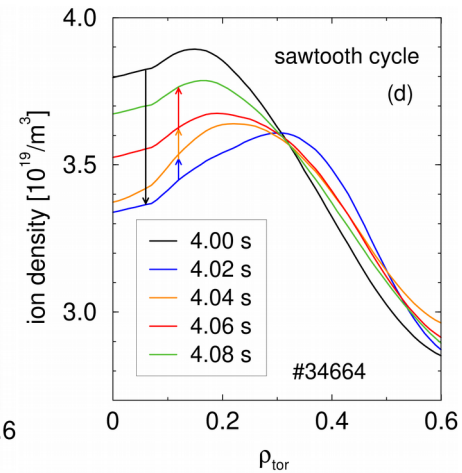
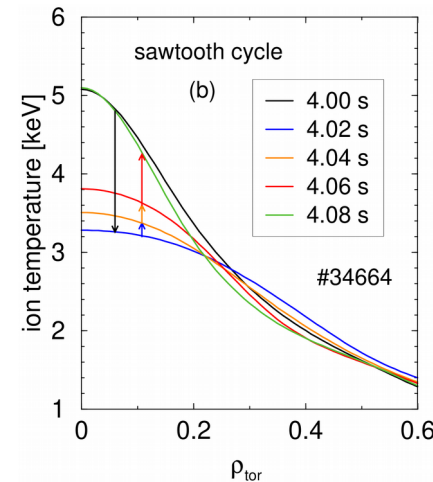
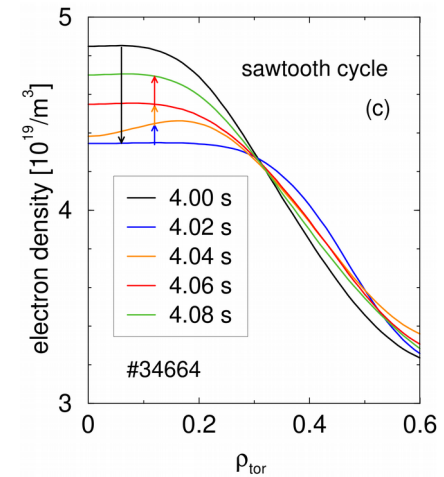
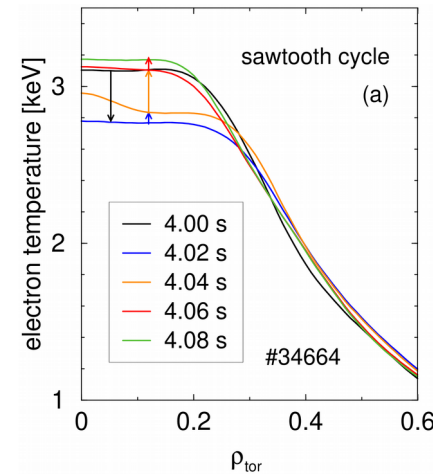
- + j_{ECCD} from TORBEAM

- + j_{NBCD} from RABBIT (Weiland NF 2018)

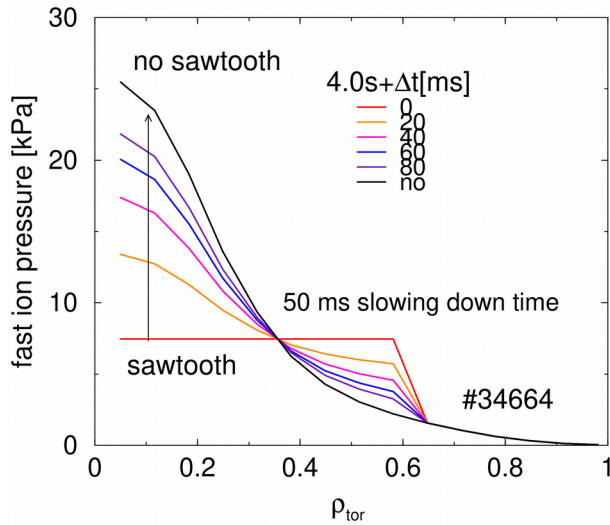
3. Sawtooth times (Gude, Maraschek)

and current relaxation model

(Kadomtsev or FCM (Fischer NF 2019))

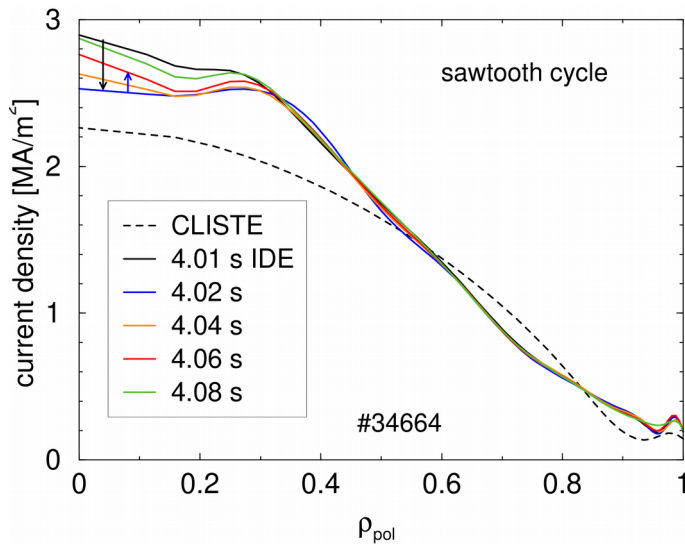
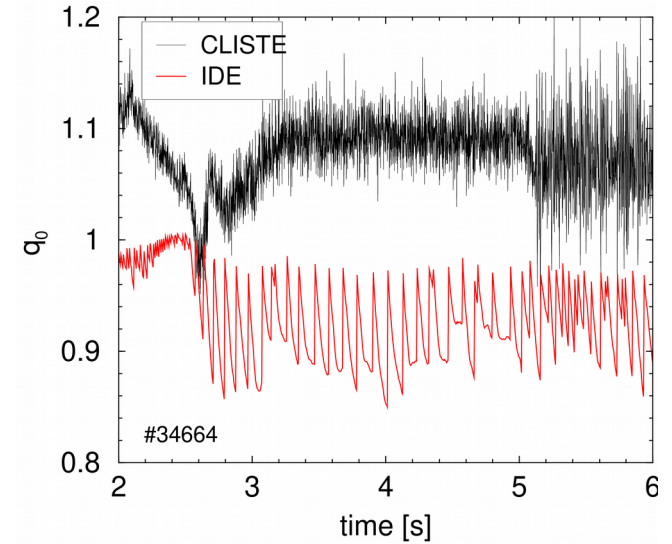


Sawtooth crash: Current redistribution



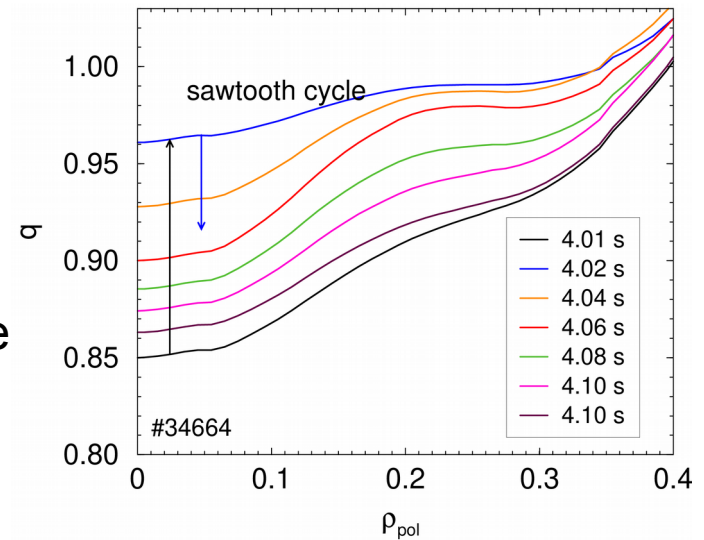
fast-ion
re-distribution

q_0 evolution



current
profile

q -profile



➤ Applications: W7-AS, JET, TJ-II, W7X, ASDEX Upgrade

Different measurement techniques (diagnostics: LIB, DCN, ECE, TS, REF, BES, HEB, ...)
for the same quantities (n_e , T_e , ...)
and parametric entanglement in data analysis (magnetic equilibrium)

➤ Probabilistic modeling of individual diagnostics

- ✓ forward modeling only (synthetic diagnostic, sensor model)
- ✓ probability distributions: describe all kind of uncertainties
- ✓ marginalization of nuisance parameters

➤ Probabilistic combination of different diagnostics

- ✓ multiply probability distributions
- ✓ systematic and unified error analysis is a must for comparison of diagnostics
- ✓ error propagation beyond single diagnostics

IDA for ITER/DEMO Improved Diagnostic Results



Bring together different **diagnostics/diagnosticians** with **redundant** or **complementary** data

- **Redundant** data:
 - more reliable results by larger (meta-) data set
→ reduction of estimation uncertainties
 - detect and resolve data inconsistencies (validation for reliable/consistent diagnostics)
using standardized error/uncertainty treatment
- **Complementary** data:
 - resolve parametric entanglement
 - resolve complex error propagation (non-Gaussian)
 - synergistic effects (exploiting full probabilistic correlation)
 - automatic *in-situ* and *in-vivo* calibration (transient effects, degradation, ...)
 - advanced data analysis technique
improvements in modelling (e.g. ECE) and diagnostics hardware (e.g. LIB)