Report on *Forward and Backward Modelling of Spectroscopic Diagnostics in Fusion Plasmas*
Doctoral thesis by Matěj Toměs, Faculty of Mathematics and Physics, Charles University

Brief summary and recommendation

As indicated by the title, this thesis describes the development and application of forward and backward models for fusion plasma diagnostic systems. Backward models are familiar to scientists performing experimental investigations, as they enable estimation of high-level plasma quantities (such as electron temperature and density) from measured data acquired by an instrument or diagnostic system. Sophisticated forward modeling is a more recent development, as it requires substantial computational power to emulate the diagnostic process and translate high-level plasma quantities into a simulacrum of measured data produced by a diagnostic system. Backward modeling has long been at the heart of experimental science, while forward modeling is beginning to be recognized as a valuable tool to ensure that diagnostic performance requirements are met with the minimum possible application of personnel and materiel.

These three diagnostic systems covered in this thesis are Thomson scattering for measurement of electron temperature and density, spectroscopic measurement of neon concentration in divertor plasmas, and camera imaging of synchrotron radiation produced by runaway electrons. The common thread linking the forward models for all three systems is application of the Raysect ray tracing engine and the Cherab framework for modeling plasma systems. The common thread linking the backward models for Thomson scattering and neon concentration is application of Bayesian statistical analysis. This backward modeling approach has the potential to increase information extraction from measured data beyond what is possible to accomplish with a frequentist approach (i.e., least-squares fitting). The three diagnostic systems in this thesis have disparate characteristics, but are linked in their need for, and benefit from, sophisticated forward and backward models.

***Recommendation**: This thesis contains new scientific results that advance fusion science and plasma physics. The author has clearly demonstrated an ability for creative and original scientific work. Therefore, I recommend that Matěj Toměs be awarded the PhD degree.*

Report written by Daniel J. Den Hartog, University of Wisconsin–Madison

Comments and questions on the thesis content

The main questions to be considered by the thesis author are presented first in the relevant sections below, and are emphasized as bullet points. These four questions should be addressed during the defense.

This thesis is written in clear understandable scientific prose. The organizational approach is appropriate for three distinct but related topics, with each main chapter written to be somewhat self-contained so that a reader interested in only one topic can read only that chapter.

Since the author of this report has more experience with Thomson scattering than the other two thesis topics, the majority of the comments and questions concern that topic.

Page numbers in the thesis are listed below as {#}.

Introduction

{6} "The contemporary trends in modeling…" This area is often referred to as "integrated data analysis." For example, see R. Fischer *et al, Plasma Phys. Control. Fusion* **45**, 1095; L. M. Reusch *et al, Rev. Sci. Instrum.* **89**, 10K103 (2018).

{8} "While the investment in advanced forward and backward modeling…" In addition, access to a fusion reactor plasma will be extremely limited, so diagnostic optimization will be critical, not just advantageous.

Forward and Backward Modeling of Thomson Scattering

- Using the results of your forward model, on what part of the COMPASS TS system would you concentrate improvement in order to further optimize diagnostic performance?
- Perhaps the earliest and most complete description of the application of Bayesian inference to Thomson scattering analysis is R. Fischer *et al*, *Plasma Phys. Control. Fusion* **44**, 1501 (2002). How does the work described in Sec. 2.3.2 advance the application of Bayesian inference to TS analysis beyond what was accomplished by Fischer and others?
- One of the steps listed on page 50 is construction of a plasma model. Does the plasma model include only an electron distribution function to produce Thomson scattering, or does it also produce other radiation (bremsstrahlung, impurity line emission, etc) that might be collected by the collection optics and recorded by the polychromator channels? Please comment on the plasma modeling choices made here.

{11} An additional advantage of a TS model for Cherab is the possibility to make design choices that minimize parasitic surface scattering of the laser beam photons into the collection optics. Such parasitic scattering makes Rayleigh calibration difficult and can overwhelm the TS signal if large and not sufficiently rejected by the polychromator channels.

{12} The direction of the electric field of the incident wave is not always perpendicular to the scattering plane. For example, see I. Yamada *et al, JINST* **7**, C05007 (2012) where the LHD TS is not sensitive to polarization orientation, or the proposal for a circularly polarized laser beam for polarimetric Thomson scattering in ITER, L. Giudicotti, *JINST* **12**, C11002 (2017).

{14} "As shown in Fig. 7 by [23], the effect of depolarization is subtle on the shape of the spectra but reduces the overall intensity of scattered radiation." This statement is correct only for scattered light collection systems that select for linear polarization parallel to the polarization of the incident wave. Not all TS collection systems contain such a selection polarizer, as the reduction in overall transmission caused by the polarizer may negate the benefit from blocking some of the background light. Also, see Fig. 2.26, in which the COMPASS core objective is shown without a polarizer.

{14} A subtle point, but check that your definition of the Selden *S* equation is normalized and integrates to unity over the epsilon variable. A colleague checked this and found that Eq. (1) in [27], $\int S(\epsilon,\theta)d\epsilon = 1.00039$, whereas $\int S(\epsilon,\theta) * (\epsilon+1)d\epsilon = 1$, which suggests $S(\epsilon,\theta)$ is normalized as a photon number distribution but defined and described as a power spectral distribution in [27].

{15} TS lasers are usually described as scientific grade rather than industrial grade, although the terms are mostly marketing speak.

{24} In Fig. 2.9, some of the measurements do not appear to have uncertainties, particularly those points in the pedestal. Are those uncertainties just small?

{26} As noted later in this thesis (page 43), a scaled Gaussian function fit to pulses with a "long tail" may not be the best procedure. The pulses are probably consistent enough that a measured model pulse including the tail might be preferable (page 60). For a detailed example of this type of approach see L. A. Morton *et al, JINST* **8**, C11003 (2013).

{27} In Fig. 2.12, what do the uncertainties represent? Specifically, do they include photon statistical noise?

{30} The comment above on integrated data analysis also applies to Sec. 2.3.2. Two additional helpful references on Bayesian inference are D. Sivia, *Data Analysis: A Bayesian Tutorial*, 2nd ed. (Oxford University Press, New York, 2002) and U. von Toussaint, *Rev. Mod. Phys.* **83**, 943 (2011).

{32} It would be preferable to define the uncertainty function $U(t)$ such that it represents only actual physical uncertainty such as expected Poisson statistical variation. Using it to help compensate for the effect of the unmodeled pulse long tail is understandable, but unsatisfying.

{35} The calibration constants $C_{p,ch,n}$ have systematic uncertainties and perhaps statistical uncertainties. A future improvement could be to include these uncertainties in the Bayesian analysis.

{35} The prior distribution selected for this analysis seems reasonable. However, care is always warranted in the selection of the form of the prior distribution and the parameters of that distribution. It is generally preferable to make the prior distribution too wide and unconstrained, as the opposite will skew the inferred values, or in the worst case, cause an important unexpected measurement to be missed.

{38} "One hypothesis is a distortion of the pulse shapes caused by electronics of the polychromator or data acquisition." Could Bayesian inference be used to test this hypothesis?

{39} "When weak evidence is present in the data, the posterior distribution starts to mirror the prior." In this case best practice may be not to plot such points since they may be misleading.

{42} A further step beyond the measurements shown in Fig. 2.20 would be use a functional form for the profile, and determine the most probable coefficients of the function.

{51} "a model approximating the bundles with a square detector with the correct acceptance angle…" It is unclear what is meant by "acceptance angle." Optical fibers are usually characterized by a core diameter and numerical aperture.

{57} This is related to the question about the plasma model. Were temperature uncertainties calculated by application of the standard least-squares codes to the forward modeled data? It seems like calculating such uncertainties would be useful when evaluating the performance of a forward-modeled diagnostic system.

{58} The caption of Fig. 2.32 refers to blue markers that "represent the relative uncertainty of profiles reconstructed from forward-modelled data." This is not uncertainty, but error as defined on page 57.

{59} Would it be practical to run a cost estimating algorithm in tandem with a diagnostic forward model? This would enable, for example, lowering measurement uncertainties by the most cost-effective means possible.

{60} The concluding paragraph on this page is well-stated. In particular, the value of forward modeling continues to need to be emphasized to the fusion community.

Neon Concentration Inference in the JET Divertor

- The need to include transport in the modeling is a recurring theme in this section. The conclusion of this section mentions that "work is ongoing on developing a more sophisticated backward model which would take into account effects of transport on the neon concentration." Please briefly describe this work and comment on the major challenges facing this effort.

{76} In Fig. 3.10, the discrepancies between the measured and forward-modeled neon line intensities are striking. Several explanations are offered in the accompanying text, but the effect of transport is not explicitly mentioned. Clarification as to whether transport might be an important factor would be helpful here.

{83} "The fractional abundances of singly and doubly ionized neon are represented by $f_{\mathrm{Ne1+}}$ and $f_{\mathrm{Ne2+}}$, respectively, and are not necessarily in equilibrium." Is transport the primary mechanism that causes a lack of equilibrium, or are there other causes?

{105} "charge exchange collisions with neutral deuterium may cause approximately 40% underestimation of the neon concentration." Would it be difficult or straightforward to include the effect of charge exchange in the model?

{106} Incorporating data from other diagnostics could be accomplished within an integrated data analysis framework.

Towards Forward Modeling of Synchrotron Radiation

{126, 129, 135} The ability of the model to provide an estimate of the effects of magnetic islands and of reflections is impressive.

{135} The approach of separating ray tracing simulations from simulations of RE dynamics is good. This type of approach should be generalized and adopted for most forward modeling.

Conclusion

{138} Forward modeling of the TS diagnostic systems on ITER would be very helpful.

{140} What of the three main topics of your thesis work should be a priority for further development?

{140} The final paragraph is a good statement of the value of the work accomplished in this thesis, and the prospects for further contributions to fusion research.

List of Publications

{156} What further publication of thesis work is planned? The publications listed here are a good start, but more material from this thesis should be published.

Typographical Errors

None of these errors are serious, but should be corrected if possible.
{7} replace → replaced
{11} "Sec." at the beginning of the text should be removed.
{15} several units of Jof energy → several Joules of energy
{47} "implementation of diverse laser profiles even pure Python functions only" (??)
{59} ambitions → ambitious; backwad → backward; appriory → a priori
{61} In the middle of the page "[.]"
{61} which goal is to provided → the goal of which is to provide
{105} Chearb → Cherab; shogood → show good
{113} Wnm−1 sr−1 → W nm^{-1} sr^{-1}
{142} Ref. [28] does not contain a complete citation. A reference to the Culham report CLM-R220?