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Promotionsverfahren von **Herrn M.Sc. Stefan Franz Walter Dasbach**  
**Auslage** der Dissertation und Gutachten sowie Termin der mündlichen Prüfung  
Anlage: Einseitige Zusammenfassung der Dissertation

Sehr geehrte Damen und Herren,

in dem oben genannten Promotionsverfahren wird die Annahme der Dissertation

**Surrogate models for particle and power exhaust in divertor tokamak simulations**

von den Berichterstattenden Prof. Dr. Y. Liang und Prof. Dr. S. Brezinsek beantragt. Sie kann zusammen mit  
den Gutachten in der Zeit

**vom 14.12.2024 bis 08.01.2025**

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Die Öffentlichkeit ist bei der Befragung zugelassen.

Mit freundlichen Grüßen  
im Auftrag

Daniela Schleiffer

## Surrogate models for particle and power exhaust in divertor tokamak simulations

The heat exhaust constitutes one of the most critical operational limits in tokamak fusion reactors. Unmitigated, the expected heat fluxes in future reactors will exceed what is sustainable for known materials. The scrape-off layer connects the plasma and reactor components. It plays a crucial role for limiting the heat fluxes to reactor components while maintaining desirable plasma conditions in the confined region. Accurate models of the scrape-off layer are required for the design and during the operation of tokamak reactors.

Simplified analytical descriptions of the scrape-off layer lack the required predictive capabilities due to a lack in the included physical processes. This often necessitates a calibration against experimental measurements, which introduces uncertainties for the planning of future larger reactors. While more complex simulations include all necessary physical processes, these simulations are computationally expensive, difficult to operate and suffer from numerical instabilities. This prevents their application in rapid design studies, algorithmic optimization or integrated modeling. A potential remedy comes in using machine learning models trained on simulations for fast and easy to use predictions. This thesis is devoted to provide a proof-of-concept of such a surrogate model and to provide recommendations for the methods to construct it.

To this end, a large dataset of several thousand SOLPS-ITER simulations using a reduced fidelity fluid neutral gas description was created. The dataset uses a conformal size scaling to encompass cross-machine scenarios across an eight dimensional parameter space. Besides the reactor size, the varied simulation parameters include the input power, deuterium throughput, impurity seeding rate and strength of anomalous cross-field transport. Analysis shows that the reduced fidelity procedure introduced some simulation artifacts, but all expected physical regimes and trends are recovered.

Based on this dataset, a variation of machine learning models with differing architectures and scopes are tested. Among these are different variants of Gradient Boosted Regression Trees and fully connected feedforward neural networks. The evaluation shows that the neural networks are the most accurate. Further, it has no benefit to develop models for specific parts of the scrape-off layer, but the conditions in the whole domain can be predicted at once. It is easier to achieve high accuracy by employing independent models for different observables rather than by using a combined model. For the tested models it is difficult to preserve the small temperature gradients in low density regimes. This leads to drastic errors in heat fluxes deduced from the surrogate predictions. Using independent models the heat fluxes can be predicted accurately but the predictions are then not consistent with the other plasma properties. So far it was not possible to create a model that predicts accurate heat fluxes self-consistent with all plasma quantities in all regimes. Analysis shows that the surrogate model accuracy drops drastically when less than 1000 training simulations are available.

Using the developed surrogate model some potential applications are demonstrated and the impurity concentrations necessary to achieve detachment are predicted for multiple tokamaks. These predictions show similar functional relations as previous scaling laws.

Finally, a small dataset of higher fidelity ITER simulations is used to train surrogate models. The smaller scope of the dataset allows for achieving much more accurate predictions. Further analysis shows that transfer learning from the previous surrogate model has no benefits over training a new model from scratch. But due to the the small number of high fidelity test simulations, no final evaluation is possible. Therefore, future efforts should focus on discovering the potential and the methods for models utilizing simulations with mixtures of fidelity.