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Fast modelling of turbulent transport in fusion plasmas using neural networks

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Accurate prediction of tokamak core plasma temperature, density, and rotation, is essential for interpretation and preparation of current-day fusion experiments, optimization of plasma scenarios, and designing future devices. Time-evolved tokamak simulation on discharge timescales is typically carried out within an 'integrated modelling'approach, where multiple models representing various physics phenomena are coupled together within a single code or workflow. An essential component of integrated models is the prediction of turbulent fluxes. In the tokamak core, transport is typically dominated by plasma microinstabilities. However, calculating these fluxes using first-principle-based nonlinear gyrokinetic models is too computationally expensive for routine simulation of tokamak discharge evolution. Reduced order turbulence models have thus been developed for increased tractability. They remain first-principle based yet are computationally cheaper by invoking the quasilinear approximation. Quasilinear turbulence models like QuaLiKiz [1,2] and TGLF 3 are approximately 6 orders of magnitude faster than δf local nonlinear codes, providing simulations on discharge timescales within the order of 100-1000 CPUh within integrated modelling. However, this remains too slow for extensive discharge optimisation and control-oriented applications.

To circumvent these conflicting constraints of model accuracy and tractability, we present an approach that leverages machine learning techniques to develop an ultrafast surrogate turbulence transport model for heat and particle transport [4]. Neural networks (NNs) are applied for regression, to learn the QuaLiKiz multivariate input-output mapping, based on a pre-calculated database of 300 million QuaLiKiz flux calculations.
The dataset generation covers a wide range of realistic tokamak core parameters. Since input space of the full QuaLiKiz code (15 dimensions for typical simulations) is too large to cover with a brute force hypercube scan, we constrain the training set dimensionality to the subset most significantly impacting turbulent transport within the framework of QuaLiKiz approximations. These input dimensions include the logarithmic ion and electron temperature gradients ($R/L_{T_{i,e}}$), density gradient (R/L_n), ion-electron temperature ratio (T_i/T_e), safety factor (q), magnetic shear ($\hat{s}$), local inverse aspect ratio (r/R), collisionality (ν^*), and effective charge (Z_{eff}), with a carbon impurity and deuterium main ion. Notable simplifications are the exclusion of plasma rotation, assuming equal density gradient for the two ion species, and no Shafranov shift. The nine inputs are taken as the feature space of the NNs. The impact of plasma rotation, which cannot be neglected, is taken into account through a new separate model in post-processing, based on $E \times B$ stabilisation and Parallel Velocity Gradient (PVG) destabilisation as determined from dedicated scans with linear-GENE [5]. A database consisting of 300 million input-flux relations was generated with HPC resources using 1.3 MCPUh. Covered regimes include Ion Temperature Gradient (ITG), Trapped Electron Mode (TEM) and Electron Temperature Gradient (ETG) turbulence. The output consists of ion and electron heat fluxes, particle fluxes, and particle transport coefficients (separate diffusive and convective terms). All outputs are dimensionless (GyroBohm units), allowing generalisation to various tokamaks.

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Regularised NNs were trained to provide an accurate and smooth regression of the QuaLiKiz dataset. Significant effort was made in ensuring the consistency of the regression with key physical features of tokamak turbulent transport. This includes sharp critical gradients for the onset of ITG, TEM, and ETG turbulent transport, maintaining the identical critical gradient for all transport channels (ion and electron heat, and particle transport), and ensuring that no spurious positive fluxes are ever predicted by the NN in regions where QuaLiKiz predicts mode stability. These constraints were achieved by customised neural network optimization cost functions, and a careful choice of regressor variables. A high quality regression was achieved, illustrated by accurate reproduction of complex structure such as ITG-TEM transitions a shown in Figure 1.

The resultant neural network transport model, QLKNN, was coupled to the tokamak modelling framework JINTRAC [6,7] and rapid control-oriented tokamak transport solver RAPTOR [8]. The coupled frameworks were benchmarked, and then validated against the original QuaLiKiz model within integrated modelling for three JET shots covering a representative spread of H-mode operating space, predicting turbulent transport of energy and particles in the plasma core. JINTRAC-QLKNN and RAPTOR-QLKNN are able to accurately reproduce JINTRAC-QuaLiKiz and , but 3 to 5 orders of magnitude faster. Simulations which take hours are reduced down to only a few tens of seconds. Further numerical optimisation is still feasible, foreseen to enable realtime predictions. The discrepancy in the final flux-driven predicted profiles between QLKNN and QuaLiKiz within integrated modelling is on the order 1%-15%. See Figure 2 for an example from JET hybrid scenario 92398. Dynamic behaviour was well captured by QLKNN, with differences of only 4%-10% compared to JINTRAC-QuaLiKiz observed at mid-radius, for a study of density buildup following the L-H transition, as seen in Figure 3.

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Following the QLKNN model development and initial validation, ongoing work focuses on extensive experimental validation of QLKNN predictions, highly facilitated by the model speed, as well as using QLKNN for scenario optimisation and design. The QLKNN model itself is currently being extended to larger input space, focusing on the impurity density gradient, and multiple-ion transport important for multiple-isotope fuelling applications and impurity transport. Additionally, using a robust method to fit a large amount of experimental kinetic profiles [10], one can base a training set on experimental data, instead of the hyperrectangle methodology described here, allowing for more input dimensions to be used. Finally, we are exploring methods to incorporate prior physics knowledge directly into the neural network architecture itself, for example by constraining the mapping to a critical gradient model. Deployment of neural network surrogate models –also beyond turbulent transport - within multi-physics integrated tokamak modelling is in general a highly promising route towards enabling accurate and fast tokamak scenario optimization, Uncertainty Quantification, and control applications.

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