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Realtime tokamak simulation with a first-principle-based neural network turbulent transport model

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Abstract:
A realtime capable core turbulence tokamak transport model is developed, extending a previous proof-of-principle (J.Citrin, S.Breton *et al.*, Nucl. Fusion **55** 092001, 2015). This model emulates a quasilinear gyrokinetic turbulent transport code, via regularized nonlinear regression using neural networks. Calculation of transport fluxes for the entire radial profile is achieved at sub-millisecond timescales. Experimental validation is presented, including ion and electron heat transport, and particle transport. The unprecedented combination of computational speed and relative modelling accuracy provided by these methods opens up enormous potential for controller design, controller validation, discharge supervision, offline operational scenario development, and application of model-based predictive control techniques.

Particle, momentum, and heat transport in the tokamak core is dominated by turbulence driven by plasma microinstabilities [1, 2]. An accurate predictive model for turbulent transport fluxes is thus vital for the interpretation and optimization of present-day experiments, and extrapolation to and control of future machines.

Nonlinear gyrokinetic simulations succeed in reproducing core transport fluxes with increasing confidence. However, the cost of such direct numerical simulation – typically 10^5 CPU hours for a single radial point – precludes the routine use of such codes for integrated tokamak transport simulations which demand $\sim 10^3$ flux computations per 1 s of plasma evolution on JET scale devices.

Quasilinear transport models are thus constructed to increase tractability. These are proven to be largely valid in the core of tokamak plasmas [3, 4, 5]. Examples are TGLF [6] and QuaLiKiz [7]. A ∼6 orders of magnitude speedup is gained in quasilinear calculations compared to nonlinear simulations. For a recent validation fo the QuaLiKiz model on a JET C-wall hybrid scenario, see figure 1. This simulation of 1 s of JET plasma evolution cost only 100 CPUh. All channels are well predicted, with the exception of inner-core T_i. This is due to the lack of ITG nonlinear electromagnetic stabilization in the QuaLiKiz saturation rule, shown to be important for this discharge [8]. Future work on QuaLiKiz will focus on this aspect.

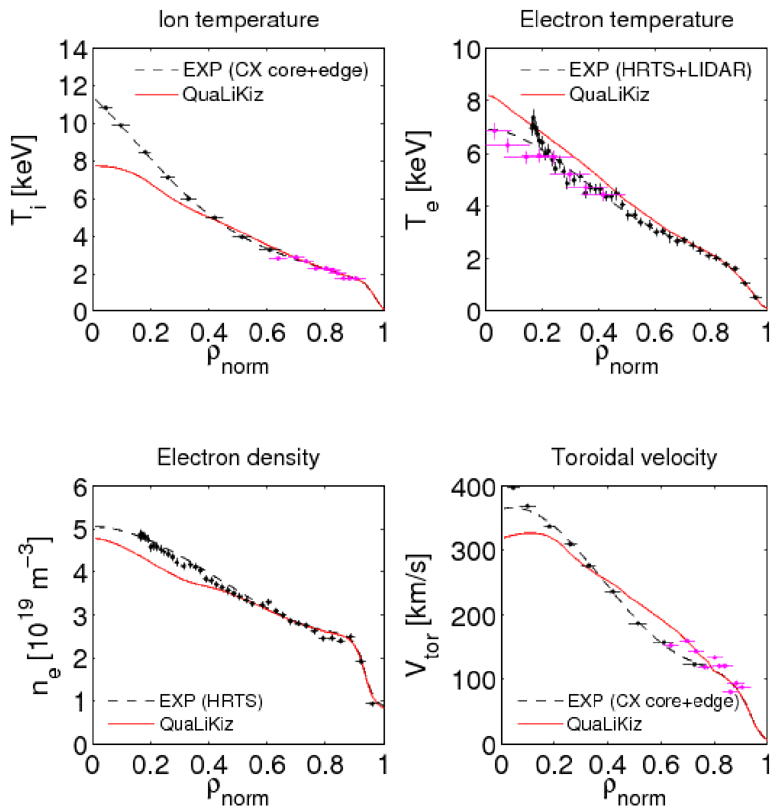

FIG. 1: QuaLiKiz simulation within the JETTO [9, 10] integrated modelling suite, of JET C-wall hybrid scenario 75225 for a time-slice averaged between 6-6.5 s. Heat, particle, and momentum transport are all simulated. Comparisons between the predictions and measurements are shown for T_i (top left panel), T_e (top right panel), n_e (bottom left panel) and V_{tor} (bottom right panel). All y-axis error bars are statistical, and are reduced due to the 0.5 s averaging. Systematic measurement errors may thus be underrepresented here.

We aim to go further, and provide a realtime-capable transport model without sacrificing model accuracy. This will open up a plethora of possibilities and innovation in realtime controller design and validation, scenario preparation, and discharge optimization. The method is based on neural network emulation of reduced quasilinear transport models. The central point is to relegate the expensive flux calculations used to train the neural network to a stage precedent to its use in a transport simulation. An extensive database of QuaLiKiz outputs is used for the neural network training.

We employ a multilayer perceptron neural network. This is essentially a nonlinear function with tunable variables (weights and biases), with the property of universal approximation [11, 12]. Neural networks have found multiple applications in tokamak research. For a summary of earlier work see Ref. [13]. Most related to this work is a regression of DIII-D heat fluxes from experimental power balance databases [14].

In the neural network, linear combinations of the inputs (e.g., for our application, local plasma parameters) and biases are propagated through a series of nonlinear transfer function vectors (named 'hidden layers'), until eventually linearly combined to an output layer. With two hidden layers and a single output value (as used in this work), this is represented as:

$$y = b_3 + \sum_{i}^{N} w_i^2 g\left(b_i^2 + \sum_{j}^{M} w_{ij}^1 g\left(b_j^1 + \sum_{k}^{I} w_{jk}^{in} x_k\right)\right) \tag{1}$$

Where y is the output 'neuron' containing the output value (e.g. ion heat flux, electron heat flux), x_k the vector of input values, b^n the bias vectors, w^{in} the M×I weight matrix connecting the input vector to the 1st hidden layer, w^1 the N×M weight matrix connecting the two hidden layers, and w^2 the weight vector connecting the 2nd hidden layer to the output neuron. g is the nonlinear transfer function, defined as a sigmoid in this work:

$$g(x) = \frac{2}{1+e^{-2x}} - 1 \tag{2}$$

The key stage is the determination of the optimized values of the weights and biases. This is done by minimizing a cost function consisting of the average squared error between the network output and known target output. This set of target output is known as the 'training set'. The BFGS algorithm [15], implementing a quasi-Newton method, was used for the weight and bias optimization. Following training, the network output then emulates the original model within the database input parameter envelope. This is validated by comparison to validation sets sifted from the database, which are different from the training set.

To avoid overfitting the data, regularization techniques were used in the regression. This corresponds to adding a penalty term in the cost function related to the sum of squares of the network weights and biases, leading to smoother output. The use of regularization ensures that the NN response is smooth (e.g. without strong oscillations) in sparse regions of training set parameter space or when extrapolating beyond the training set envelope.

The analytic form of the nonlinear regression function allows for the calculation of analytical gradients of the outputs with respect to the inputs. This is vital for the efficient solution of fast implicit schemes in real-time capable core transport simulators such as

TABLE I: Summary of input parameters for the QuaLiKiz ITG database employed in this work

Parameter	Min value	Max value	No. of points
R/L_{Ti}	2	12	30
T_i/T_e	0.3	3	20
q	1	5	20
$\hat{s}$	0.1	3	20
$k_\theta \rho_s$	0.05	0.8	16
Total no. of points			3 840 000

RAPTOR [16]. The regularization also ensures smooth gradients throughout parameter space, important for the stability of such implicit schemes and for trajectory optimization applications.

A database of QuaLiKiz solutions was constructed, in the ion temperature gradient (ITG) instability regime. This instability is often the primary driver of tokamak micro-turbulence. The database covers four input parameters known to have significant impact on ITG transport fluxes in this regime: the driving normalized logarithmic ion temperature gradient R/L_{Ti}, the ion to electron temperature ratio T_i/T_e, the safety-factor q, and the magnetic shear $\hat{s} \equiv \frac{r}{q}\frac{dq}{dr}$. In addition, the input normalized wavenumber $k_\theta \rho_s$was scanned, constricted to above ion-Larmor-radius scales, where $\rho_s \equiv \sqrt{T_e m_i}/(Z_i q_e B)$. The following parameters were maintained fixed: the normalized logarithmic density gradient $R/L_n = 3$, normalized radial location $r/a = 0.5$. No Shafranov shift was assumed in the geometry. The database consists of a dense grid of points summarized in table I, from which the training sets for the neural network were sifted. The QuaLiKiz outputs we investigate are: ion heat flux, electron heat flux, electron particle diffusion, and electron particle pinch. An adiabatic electron version of this same database was previously carried out [17] (and thus limited to only ion heat flux). Here, we extend the database to kinetic electron cases.

To capture the instability thresholds with high fidelity, the regression was only carried out for a training set corresponding to unstable modes. The NN output for the stable regions in the validation set was then negative, since the regularized network tends to smoothly extrapolate the trends observed towards the training set envelope. For the final flux outputs, these negative values were then set to zero to represent stability. This scheme avoids having the regularized regression network attempt to directly fit the discontinuous gradients at the instability thresholds, which would be performed poorly due to to the regularization constraint. This is an important point since tokamak transport often tends to be maintained near the critical temperature gradient thresholds, especially in high temperature regimes.

The typical quality of the fits can be seen for the ion heat conductivity in figure 2, displaying scans of the 4 separate input parameters while the others remained fixed. Negative outputs of the NN network are set to zero. Note the resulting excellent fit of the instability thresholds. In addition, extrapolating the NN scans beyond the range of the training set maintains the trend observed in the data, due to the regularization. This is very encouraging with regard to extension of this approach to more sparse datasets in higher dimensions. However, we do not intend to routinely use NN models in poorly represented regions of parameter space, as the quality of extrapolation cannot be determined a priori. Rather, the training sets should be continuously expanded to cover such encountered sparse or empty regions, and the NN then periodically retrained. Nevertheless, the smoothness of the regularized NN response when extrapolating ensures its robustness and stability during practical use as a transport model, including during phases when such sparse regions are encountered.

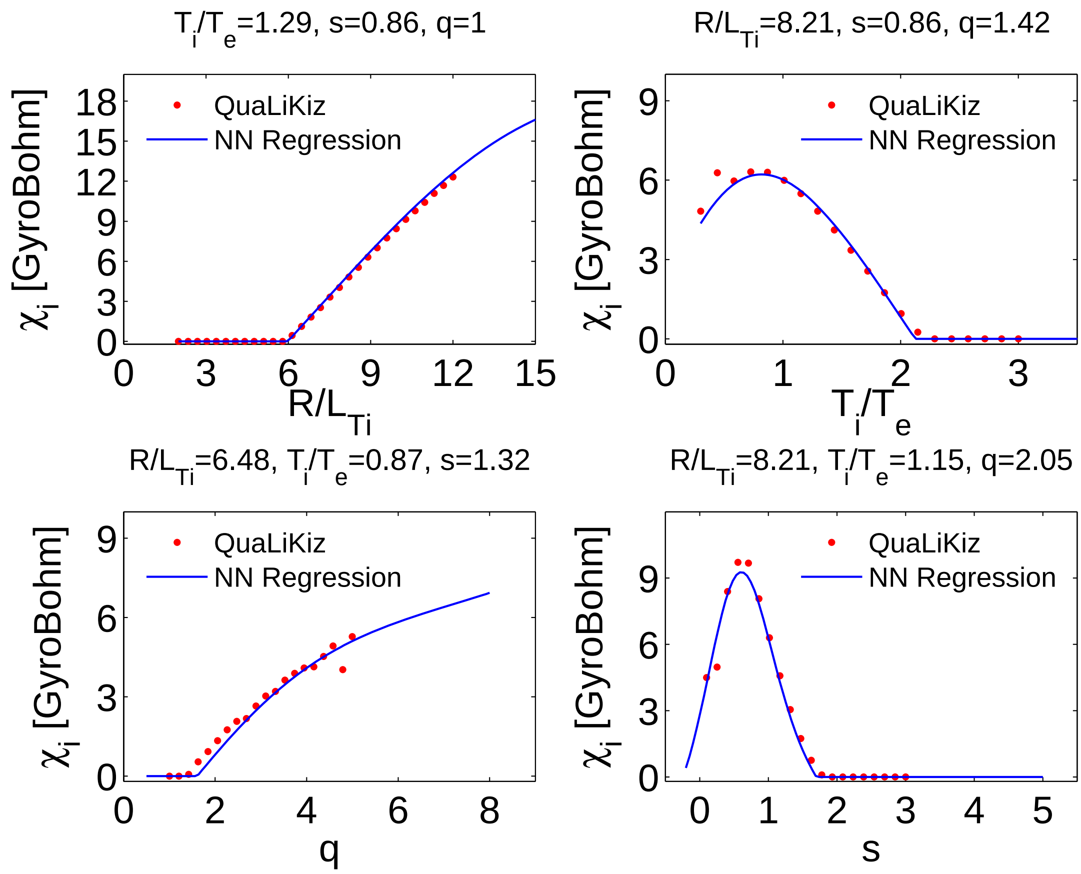

FIG. 2: Comparison of NN parameter scans (blue solid lines) vs the original QuaLiKiz ion heat flux calculations (red dots). The scans are in R/L_{Ti} (top left panel), T_i/T_e (top right panel), q (bottom left panel) and $\hat{s}$ (bottom right panel). This is for the adiabatic electron case, and the plot is from Ref. [17]

Each NN output is calculated on a sub 10 μs timescale in MATLAB on a Intel(R) Xeon(R) E5450 CPU @ 3.00GHz. This is a 6 order of magnitude speedup in comparison to the original QuaLiKiz calculations.

A transport model based on the trained neural network was constructed, and implemented both in the CRONOS [18] and RAPTOR [16] integrated modelling codes.

In CRONOS, the validity of the NN transport model was assured by a successful comparison with a JET baseline H-mode shot 73342 with ion and electron heat transport previously simulated [19] with the full QuaLiKiz model. This is shown in figure 3. The level of agreement is extremely encouraging, especially considering that only a reduced dimensionality ITG QuaLiKiz database was used for the neural network training.

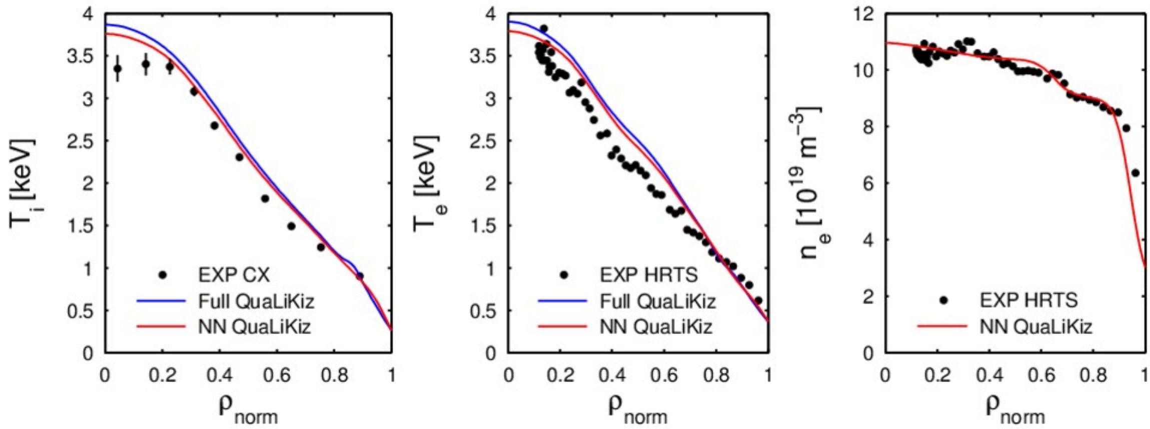

FIG. 3: Comparison between T_i (left panel), T_e (center panel), and n_e (right panel) predictions of the original QuaLiKiz model (blue curve) and the NN regression (red curve), corresponding to JET shot 73342 at 10.1 s, modelled in CRONOS with self-consistent heat source calculations.

We now focus on realtime applications within RAPTOR. In figure 4, we compare a RAPTOR simulation of an ITER hybrid scenario, using the QuaLiKiz NN model for electron heat transport, with a simulation of the same case originally carried out [20] using CRONOS and the GLF23 [21] transport model. Using GLF23 allows to compare over ITER-scale discharge times of >100s, which is less tractable using the original QuaLiKiz model. For heat transport in a pure ITG regime, GLF23 and QuaLiKiz predictions are expected to be similar, as illustrated in specific single-time-slice comparisons [19].

The RAPTOR simulation uses all the same actuator (source) inputs and density evolution as the CRONOS simulation. Ion temperatures were held fixed at $T_i/T_e \sim 0.8$ in L-mode and $T_i/T_e \sim 0.9$ in H-mode. The NN model was operational within a normalized toroidal flux coordinate (ρ) range of 0.25 to 0.95. For $\rho > 0.95$, χ_e was feedback controlled to maintain a prescribed edge pedestal temperature of 4 keV. For $\rho < 0.25$, a constant χ_e was assumed to maintain a reasonable level of transport, since GLF23 and QuaLiKiz both predicted stability within that region. A RAPTOR simulation of an entire 300 s ITER discharge took 10 s on a single CPU, corresponding to 30x faster than real-time. This combination of simulation speed and first-principle modelling is unprecedented. With CRONOS/GLF23, the same simulation took 24 hours.

For the next stage, moving beyond this proof of principle, a higher input dimensionality QuaLiKiz database is currently under construction. This contains a 10D hypercube of input parameters consisting of $k_\theta\rho_s$ (ion and electron scales), R/L_{Ti}, R/L_{Te}, R/L_n, q, $\hat{s}$, r/R, T_i/T_e, Z_{eff}, and collisionality. All ranges are based on typically encountered experimental parameters. A Be impurity will be assumed, and the density gradients of all species kept equal. The neural network fit of this database will thus capture the physics of ITG, TEM, and ETG turbulence, and be valid in more general regimes than our current

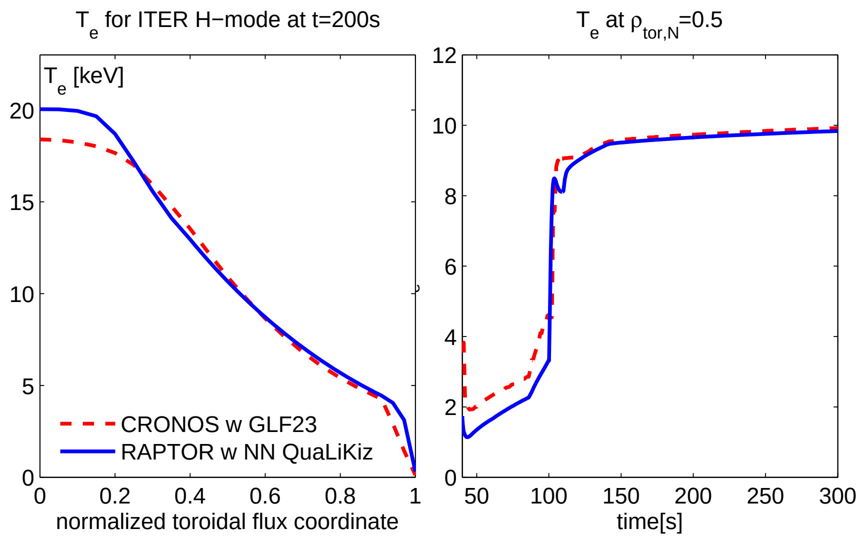

FIG. 4: Comparison between the T_e predictions for an ITER hybrid discharge carried out with CRONOS/GLF23 [20] (red curve) and a RAPTOR simulation using the QuaLiKiz NN transport model (blue curve). A typical H-mode profile (left panel) and time dependence at mid-radius (right panel) are shown. The LH transition was set at 100 s.

proof of principle. The I/O and nonlinear saturation rule in QuaLiKiz has been more extensively parallelized in preparation for this work, to allow for efficient operation with large run sizes on HPC architectures.

To summarize, a neural network fit to a restricted subspace of quasilinear gyrokinetic transport model calculations, relevant in the ITG regime, was carried out and applied as a transport model for integrated modelling. While the quasilinear model, QuaLiKiz, is 6 orders of magnitude faster than nonlinear simulations, the NN regression leads to a further 5 order of magnitude speedup. This model is thus real-time capable while still being based on first-principles, which is unprecedented. This model has been coupled to the CRONOS integrating modelling suite, and validated against a full QuaLiKiz simulation in the ITG regime. The model is also coupled to the real-time capable RAPTOR tokamak simulation code, and can model a 300s ITER discharge within 10s, with good agreement with previous modelling using CRONOS and the GLF23 transport model.

This opens up many new possibilities for real-time controller design and validation, scenario preparation and optimization, and real-time discharge supervision. Such models can be used to design controllers for the plasma profiles using model-based controller design methods (e.g. [22] or [23]). The transport model can be used in closed-loop simulations to validate the designed controllers. Recent work on plasma ramp-up trajectory optimization [24] was carried out with an ad-hoc transport model, and can now be improved using this first-principle-based transport model. Also, this transport model can be used in real-time simulations to verify the measured plasma evolution and warn a supervisory control system of any unexpected deviations during the discharge [25]. Specifically for ITER, the faster-than-real-time opens up the possibility of (on-line) real-time optimization of the discharge evolution in response to such unexpected events.

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