Realtime capable first principle based modelling of tokamak turbulent transport

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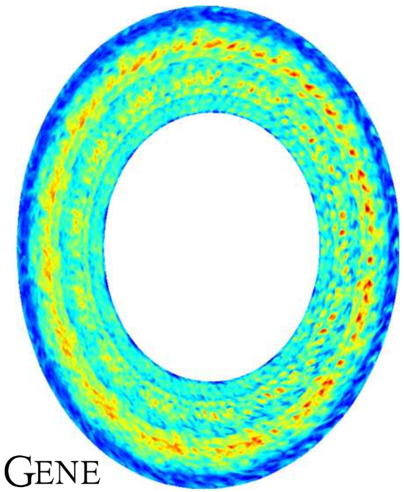
Motivation

- For realtime control, a tokamak simulator must calculate turbulent fluxes on <ms CPU timescale!
- No such first-principle-based model currently exists
  How to combine tractability and accuracy?
- Would allow (among others):
  i) efficient offline tokamak scenario preparation and optimization
  ii) discharge supervision
  iii) realtime trajectory optimization

Model hierarchy: 'The Gold Standard'

1st reduction:
gyrokinetics (5D), local (spectral radially), δf splitting, gradient driven



e.g., GS2/GYRO/GENE/GKV etc etc etc...

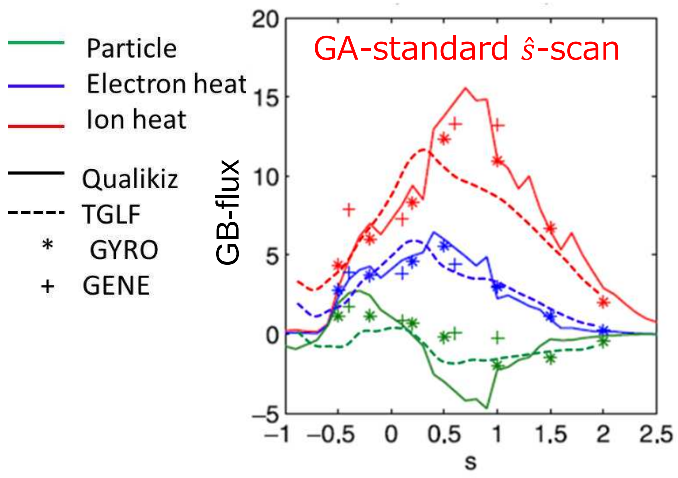
- Calculation of fluxes at one radial point within **10^4-10^5 CPUh** (ion and electron scales seperately)
- Allows electromagnetic fluctuations, multiple ion species, collisions
- Validated flux matched simulations vs dozens of experimental cases
- We consider this the 'gold standard' for validating reduced models further down the hierarchy

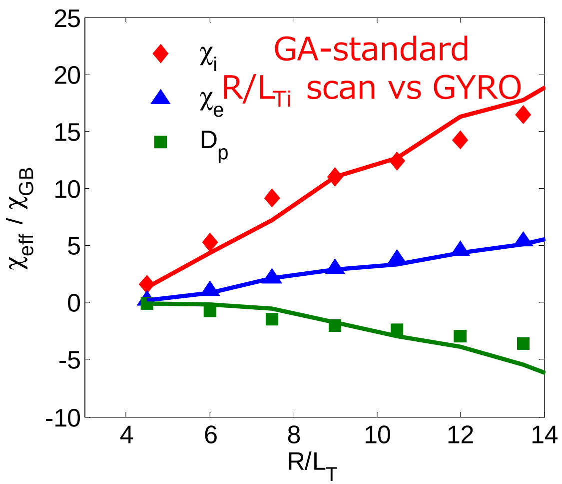
2^{nd} reduction: quasilinear modelling

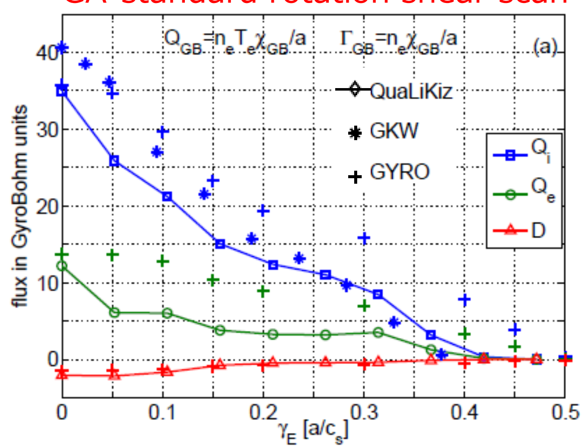
2nd reduction: quasilinear, e.g. gyrofluid TGLF (G. Staebler PoP 2008) gyrokinetic QuaLiKiz (C. Bourdelle PoP 2007),

$$\Gamma, \mathrm{Q}, \Pi = \sum_k (\delta n, \delta T, \delta v_\parallel\ modified\ linear\ response) \cdot S_k |\delta\phi_k|^2$$

Key point: $\delta\phi_k$ spectral form and nonlinear saturated amplitude prescribed based on physical motivations and fits to nonlinear simulations from up the hierachy







Following recent speedups (JC TTF 2014, paper in progress)
~ 1 CPUs to calculate flux at single radial location. 10^6 faster than nonlinear

Reduced reduced reduced modelling...

$1\ CPUs$ is fast but not fast enough for realtime control!
How can we go further?

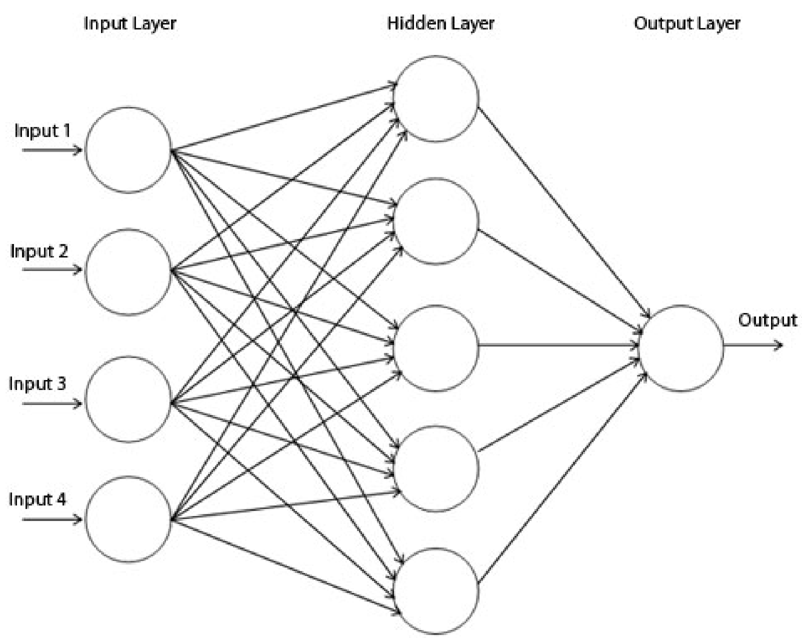
1. Obtain a good quasilinear model validated vs nonlinear simulations
2. Use quasilinear model to create enormous datasets of turbulent flux calculations. Include all tokamak parameters of interest (e.g. based on experiments). Feasible with 10^7 CPUh scale HPC projects (currently 'routine')
3. Define 'training sets' from the database to construct nonlinear regressions of the data.
4. Use the fitted nonlinear regression as the 'transport model'

The nonlinear regression technique we've been exploring is
Multilayer Perceptron Neural Networks

Successful and similar recent work:
neural network fit of DIII-D power balance fluxes with ~20D input space (Meneghini PoP 2014)

Explanation of neural network technique

Multilayer perceptron network: nonlinear mapping



Inputs: e.g. T_i/T_e, q, $\hat{s}$, R/L_{Ti}

Each node output in "hidden layer": nonlinear function of linear input combination

$$g_j = g\left(\sum_i w_{ij} x_i\right)$$

With, e.g. $g(x) = \dfrac{2}{1+e^{-x}} - 1$

Universal continuous function approximator (basic literature, Bishop 1995, Haykin 1999)

- Optimal weights found in off-the-shelf optimization algorithms from 'training set' of known input-output relations
- The trained network then generalizes to previously unknown inputs
- Regularization techniques important to avoid overfitting
- Trained network output in <ms, orders of magnitude less than original calc.
- In the end, an analytical formula with defined analytical derivatives. Critical for trajectory optimization and implicit timestep solvers

A proof-of-principle NN transport model

Neural network fit for QuaLiKiz output. Adiabatic electrons. ITG regime

(JC, Sarah Breton, F. Felici, F. Imbeaux, accepted to Nucl. Fusion Lett.)

5D input space: q, $\hat{s}$, T_i/T_e, R/L_{Ti}, $k_\theta \rho_s$

Outputs: growth rates, frequencies, ion heat flux

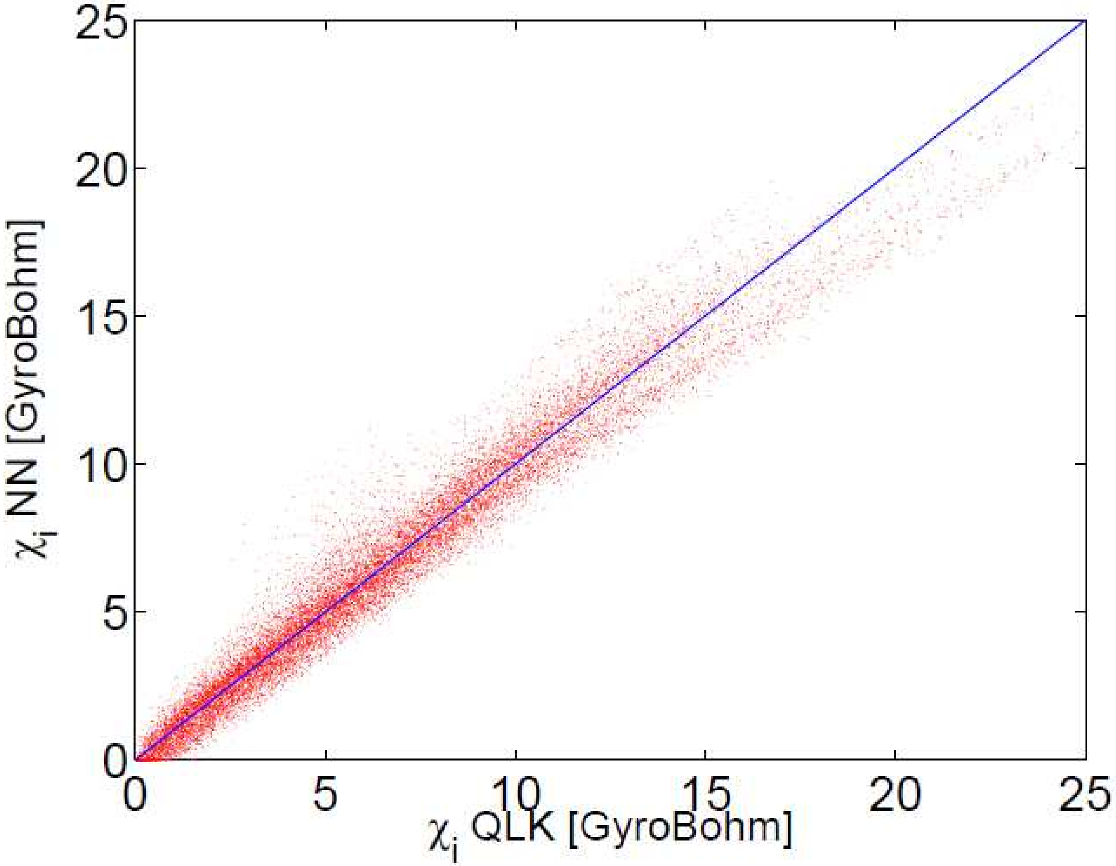
~4 million instability calculations (4 processors, 1 week). Dense 5D array

q = 1-5, s = 0.1-3, Ti/Te = 0.3-3, R/Lti = 2-12, $k_\theta \rho_s$ = 0.05-0.8 (ion scales)

- Training and validation sets are cut from this large total sample set
- Only ~50,000 points necessary in training set for robust fit
- Regularization avoids overfitting and even allows some extrapolation

Comparison of neural network fits

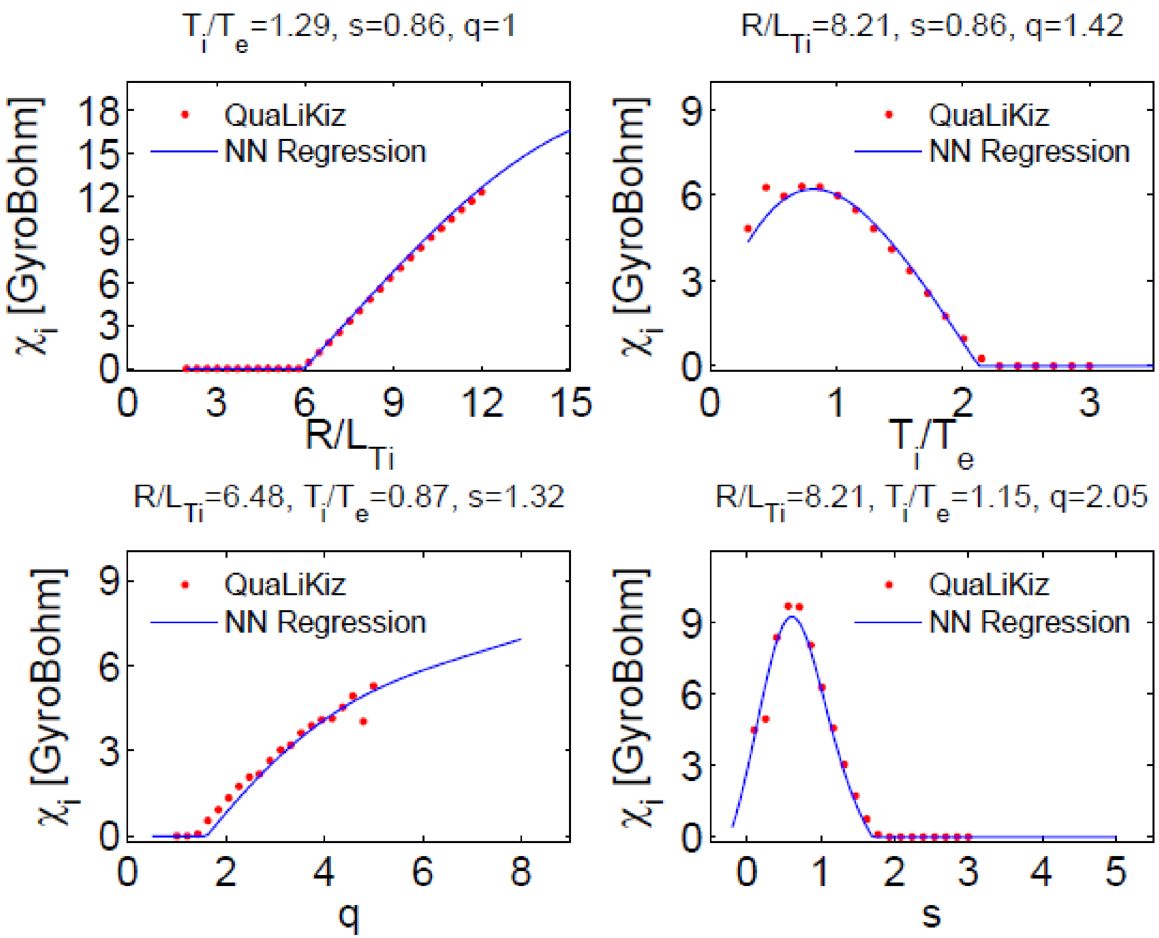
Comparison between fitted network and original model



RMS error of ~0.8 in GB units. Most discrepancies are due to regularization, not inherently poor fitting.
Propagates to small $\Delta R/L_{Ti}$ errors (~0.4) due to stiffness

Comparison of neural network parameter scans

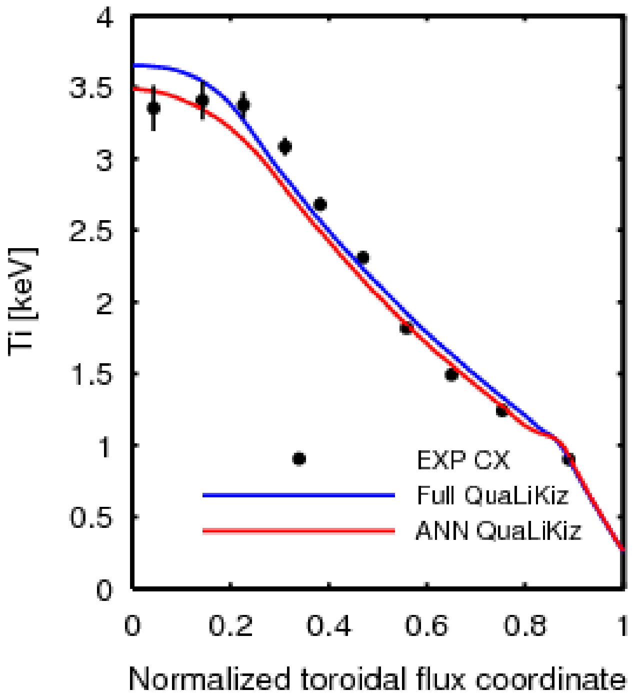
Parameter scans of NN ion heat conductivity vs original QuaLiKiz results

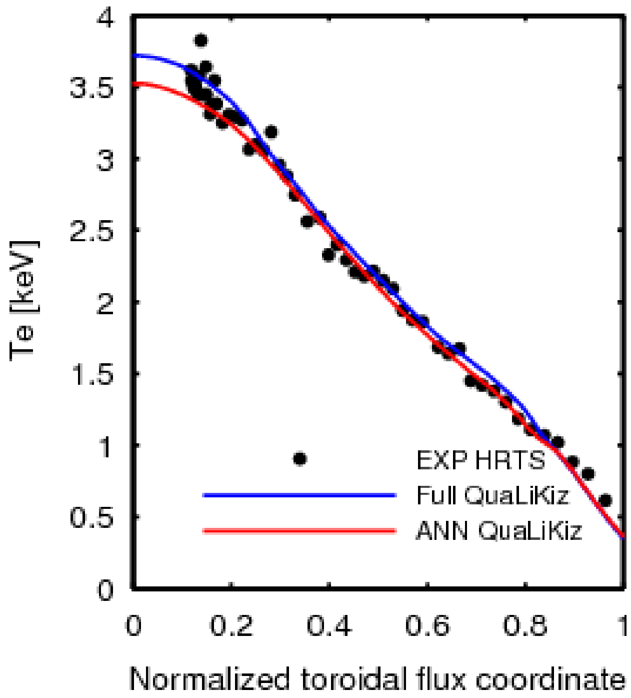


Note that regularization allows reasonable extrapolation.
Extrapolation not recommended, but encouraging for robustness in sparse datasets

Successful results even with basic 'proof-of principle model' in ITG regime

- QuaLiKiz NN regression now a transport model in CRONOS integrated modelling code
- Comparison made to QuaLiKiz simulation (Baiocchi NF 2015) of JET 73342





Excellent agreement

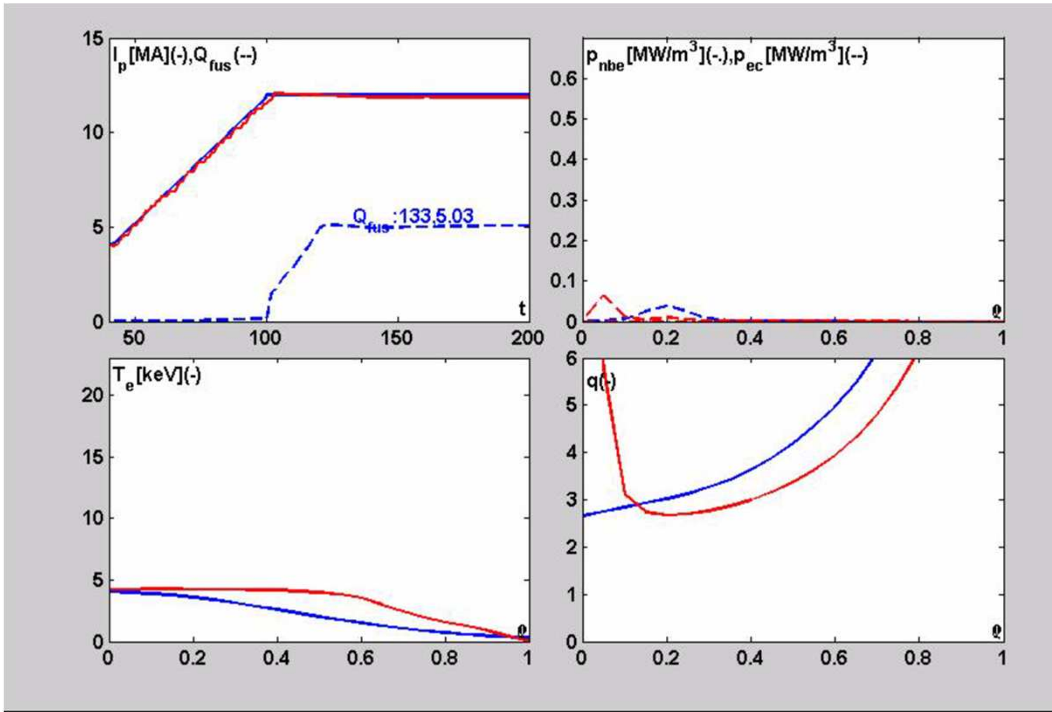
Full profile transport fluxes calculation only 0.5 ms with 1 CPU with neural network.
Factor $10^5 – 10^6$ speedup!

Simulation with NN took 10 mins with 1 CPU instead of 1 day with 24 CPUs!

Fluxes were not the bottleneck in calculation

Realtime transport model in RAPTOR

- QuaLiKiz neural network applied in ultra-fast RAPTOR simulator (F. Felici et al 2012)
- Extrapolation to ITER hybrid scenario. QuaLiKiz ANN compared with GLF23 modelling (JC NF 2010). (GLF23 gyrofluid quasilinear model valid in ITG regime)
- QLKANN/RAPTOR took 8s to calculate 300 ITER seconds!
  GLF23/CRONOS took 1 week for same calculation (on 1 CPU)



BLUE – QLK Neural Network. RED – GLF23

Summary

- Set out on a quest for simultaneous accuracy and tractability in turbulent transport models in tokamaks
- Key technique: neural network regression of a quasilinear reduced model, itself validated by nonlinear gyrokinetics
- First proof-of-principle 5D network created and applied in transport models. Can reproduce QuaLikiz and GLF23 ITG heat transport

Perspectives

- Extensions to much higher QuaLiKiz input dimensions ongoing for more generality and instability branches (MSc project Juan Redondo)
- Use more complete (but slower) solvers than QuaLiKiz/TGLF (e.g. linear-GENE/GKW/GYRO) for high accuracy in the training sets
- Validate RAPTOR/QLKANN output vs experimental data.
Explore trajectory optimization, including with particle transport
- Set up a community-wide linear database with standardized I/O.
Pool resources for training sets. Very useful for benchmarks.
Not dependent on nonlinear saturation rules which continuously evolve
- Extend nonlinear regression techniques to other models. e.g. pedestal stability (EPED), neoclassical transport, MHD stability limits.
Ambition: a <u>realtime</u> integrated tokamak simulator from first principles