Multi-channel flux driven simulation with the quasilinear gyrokinetic tokamak transport model QuaLiKiz

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**See the Appendix of F. Romanelli et al., Proceedings of the 25th IAEA Fusion Energy Conference 2014, Saint Petersburg, Russia*

Full integrated tokamak modelling demands tractable calculations of all components

Full prediction and optimization cannot be inferred from the isolated behaviour of the components

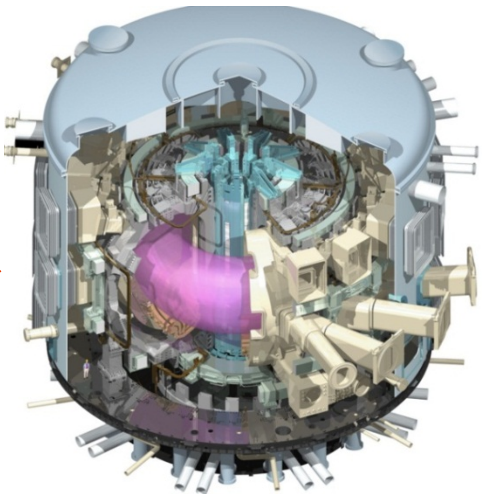
Magnetic equilibrium

Heating

MHD stability

Turbulence

Plasma-wall-interaction



Fusion power

Heat exhaust

Calculation of each physics component must be reduced to a tractable level

Profile evolution of thermodynamic quantities limited by turbulent fluxes

1D core profile evolution

Particle flux | Particle sources/sinks

Particle density: $$\frac{\partial n_s}{\partial t} + \frac{\partial}{\partial r}(\Gamma_s) = S_s$$

Energy: $$\frac{3}{2}\frac{\partial P_s}{\partial t} + \frac{\partial}{\partial r}(q_s) = Q_s$$

Heat flux | Heat sources/sinks

CRONOS
ETS
JETTO
PTRANSP
ASTRA…

$$t_{integrated\ sim.} = \boldsymbol{t_{turb.fluxes}} \times N_{radial\ points} \times \frac{t_{discharge}}{\Delta t_{PDE\ evolution}} \times N_{iterations}$$

$$t_{integrated\ sim.} \approx \mathbf{10^5} \times \boldsymbol{t_{turb.fluxes}}$$

Large number of calls to turbulent transport model

Turbulent flux calculations are expensive. Significant approximations -> profile evolution

Aim at: $\mathrm{t_{integrated\,sim.}} \approx 10^5 \times \mathbf{t_{turb.fluxes}} < \mathbf{24\,h}$ on ~30 CPU, hence need $\mathbf{t_{turb.fluxes}} \sim \mathbf{10\,s}$ for ~10 $k_\theta \rho_s$ on 1 CPU

Local gyrokinetics, e.g. **GS2** [Kotschenreuther PoP95], **GENE** [Jenko CPC00], **GYRO** [Candy-Waltz JCP03], **GKW** [Peeters CPC09]		Local gyrokinetic code with additional approximations: **QuaLiKiz** [Bourdelle, Garbet et al PoP07, PPCF 16]
Non-linear	Quasilinear	
~ 50 000 h	~ 100 h	~ 10 s

Other quasilinear codes with $\mathrm{t_{turb.fluxes}} < \sim 1\,\mathrm{min}$:

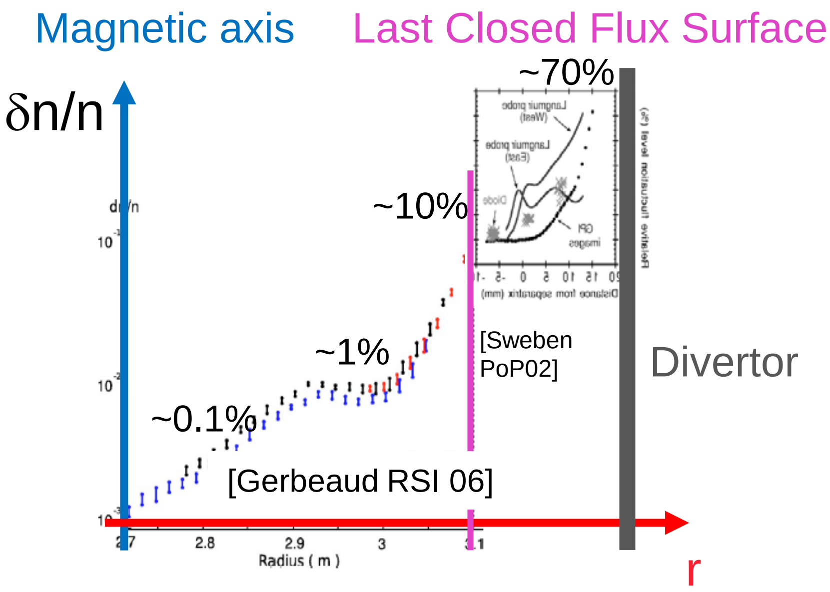
- Weiland-MMM [Weiland NF89, Rafiq PoP13] fluid model
- GLF23 [Waltz PoP97] and TGLF [Staebler PoP07] gyro-Landau fluid model

Outline

- Overview of the QuaLiKiz model
- What’s new? Model improvements and physics generalizations recently applied
- JET experimental validation of density, temperature and rotation profiles prediction with QuaLiKiz
- A neural network QuaLiKiz for realtime modelling

Quasilinear transport models justified from measurements and nonlinear simulations (1)

In tokamak core, reflectometry measurements: $\delta n/n < 10\%$

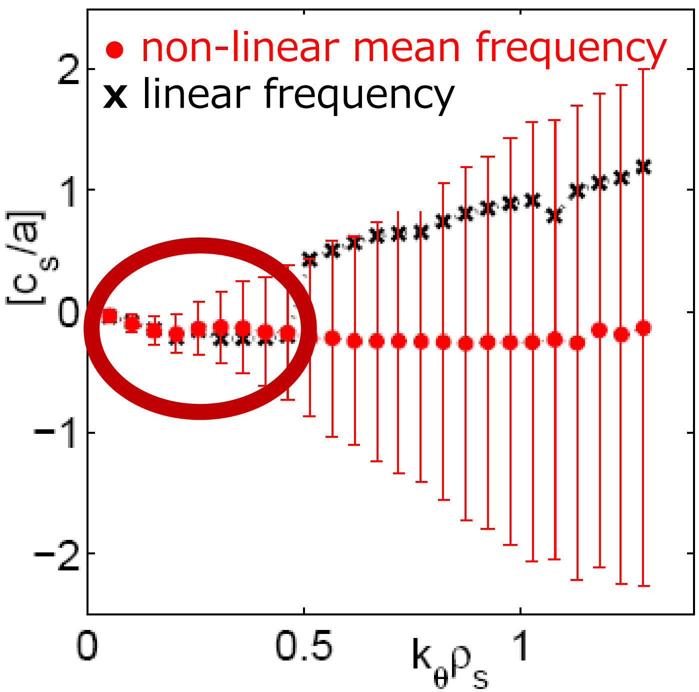


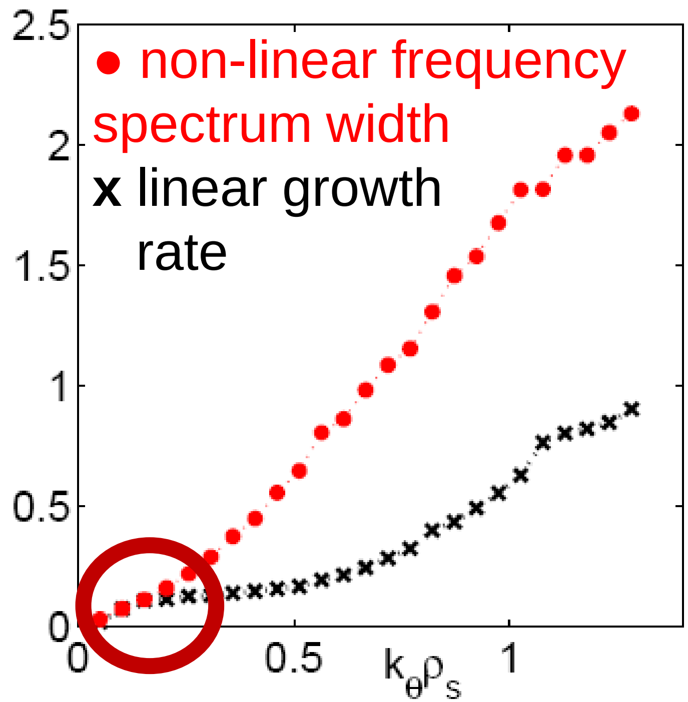
→ can assume $\delta n \ll n$

Motivates linearisation of Vlasov equation, and suggests weak nonlinearity

Quasilinear transport models justified from measurements and nonlinear simulations (2)

In wavenumber range that drives most transport ($<0.5\, k_\theta \rho_s$), nonlinear simulations shown strong signatures of underlying linear modes



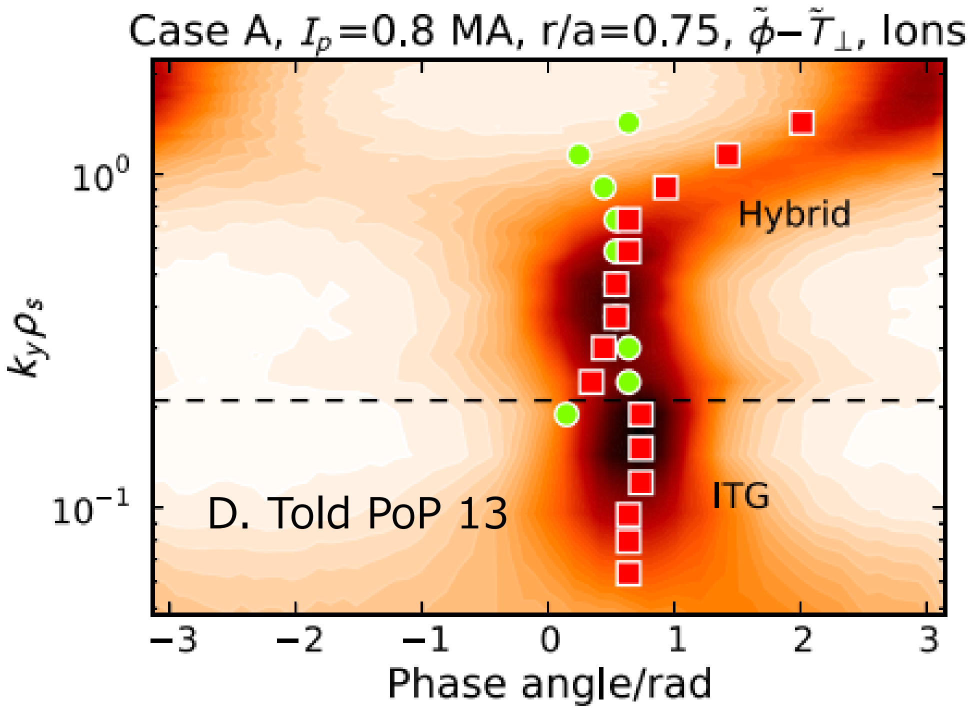


GYRO linear and non-linear of TS39596 at r/a = 0.7 [Casati 2009 PhD]

[Dannert PoP05, Lin PRL07, Merz PRL08, Casati NF09]

NB: for |s|<0.6 need ad-hoc adjustment for frequency broadening [Citrin PoP2012]

Quasilinear transport models justified from measurements and nonlinear simulations (3)



Relative phase comparison (cross-phase) between $T_\perp$ and electrostatic potential fluctuations

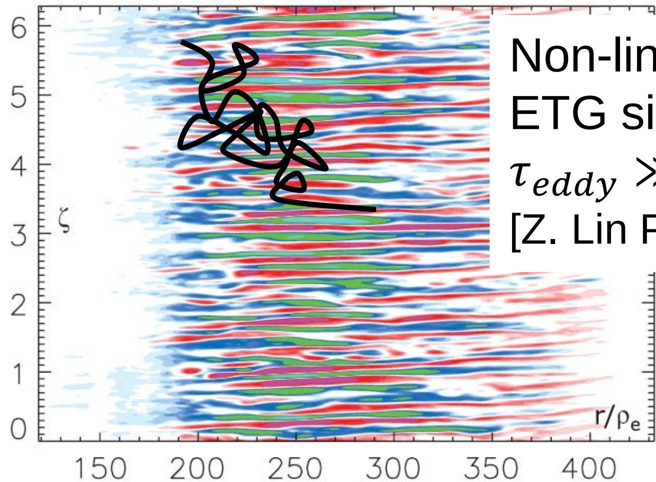
GENE nonlinear simulation of AUG discharge

Can consider tokamak turbulence in transport driving ranges:
"Bath of linear-like fluctuations whose amplitude and exact wavenumber spectra are set by nonlinear physics"

Linear fluctuation characteristics are not washed out of nonlinear system

Quasilinear transport models justified from measurements and nonlinear simulations (4)

In core, wave-particle decorrelation time < eddy turnover time. No field trapping
[Casati NF09, Citrin PoP12]



Non-linear global ETG simulation
$\tau_{eddy} \gg \tau_{"flight"}$
[Z. Lin PRL07]

i) Kubo number < 1 (and of O(1))
ii) Recall: $\Delta\omega_{nonlin} \approx 1/\tau_{decorellation} \sim \gamma_{lin}$ at each wavenumber

Together, motivates random walk diffusion model with $D_k \propto \frac{\gamma_k}{k_\perp^2}$
(forms part of nonlinear saturation rule in QuaLiKiz)

Sketch of QuaLiKiz model construction (1)

$$\frac{\partial f_s}{\partial t} + \boldsymbol{v} \cdot \nabla_{\mathrm{r}} \mathrm{f_s} + \mathrm{e_s} \mathbf{E} \cdot \nabla_v f_s = 0$$

Electrostatic Vlasov (collisionless here for simplicity)

$$\delta f_s(\omega, k) = \frac{F_M}{T_s}\left(1 - \frac{\omega_k - n\omega_s^*}{\omega_k - k_\parallel v_\parallel - n\omega_{sD}}\right) e_s \phi_k$$

Linearized Vlasov with harmonic perturbations

$$\sum_s \int d^3v d^3x \, \delta f_s e_s \phi_k^* = 0$$

Weak form for quasineutrality to close dispersion relation

Sketch of QuaLiKiz model construction (2)

Dispersion relation: passing, trapped, trapped electrons

$$D(\omega)=\sum_s \int dr d\theta d\lambda d\epsilon \, \frac{n_s e_s^2}{T_s}\left(1-\frac{\omega_k - n\omega_s^*}{\omega_k - [k_\parallel v_\parallel, 0] + i\nu - n\omega_{sD}} J_0^2(\mathrm{k}_\perp[\rho_s,\delta_s])|\delta\phi(r,\theta)|^2\right)=0$$

$$k_\parallel = k_\theta \frac{s}{qR} x$$

From eikonal: $\delta f, \delta\phi \propto \mathrm{e}^{-\mathrm{in}(\varphi - \mathrm{q(r)}\theta)}$

x≡distance from q surface

ϕ eigenfunction solved from high ω expansion of D(ω) and Gaussian ansatz

$\omega \equiv \omega_r + i\gamma$ is the only unknown in the above equation.
Root finding in upper complex plane (instabilities only)

Setting quasilinear fluxes with a nonlinear saturation rule

Transport fluxes for species j: carried by ExB radial drifts

$$(\Gamma_j, Q_j, \Pi_j) \propto \sum_k \langle (\delta n_j, \delta T_j, \delta v_\parallel) \times S_k \delta\phi_k \rangle$$

Use moments of linearized δf_s evaluated at the instabilities, i.e. from solutions of $D(\omega_k)$

Spectral form factor S_k and saturated amplitude of $|\delta\phi|^2$ are unknowns. Their model, validated by nonlinear simulations, is the "saturation rule"

$$S_k \propto \begin{cases} k^{-3} \; for \; k > k_{max} \\ k \; for \; k < k_{max} \end{cases}$$

$$k_{max} \; is \; k \; at \max\left(\frac{\gamma_k}{k_\perp^2}\right)$$

$$|\delta\phi_k|^2 = C S_k \max\left(\frac{\gamma_k}{k_\perp^2}\right)$$

Casati NF 09, PRL 09

C is scalar factor set by matching heat fluxes in single NL simulation (for ion and electron scales separately)

$$< k_\perp^2 >= k_\theta^2(1+s^2 < \theta^2 >)$$

+ finite k_x corrections at low-s from nonlinear physics (JC, PoP 2012)

QuaLiKiz fast calculation time due to significant assumptions made (1)

QuaLiKiz assumptions

- Ballooned Gaussian eigenfunction ansatz
- Averaged $\langle k_\parallel v_\parallel \rangle, \langle \omega_d \rangle$ instead of full passing species pitch angle integration
- Shifted circle $(s-\alpha)$ geometry
- Electrostatic only
- Collisions only with Krook operator for trapped electrons

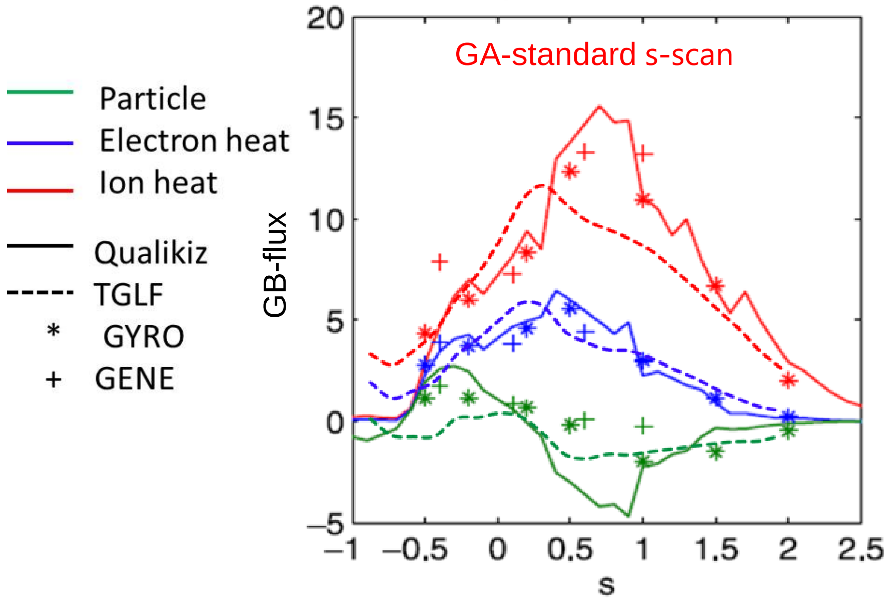
QuaLiKiz fast calculation time due to significant assumptions made (2)

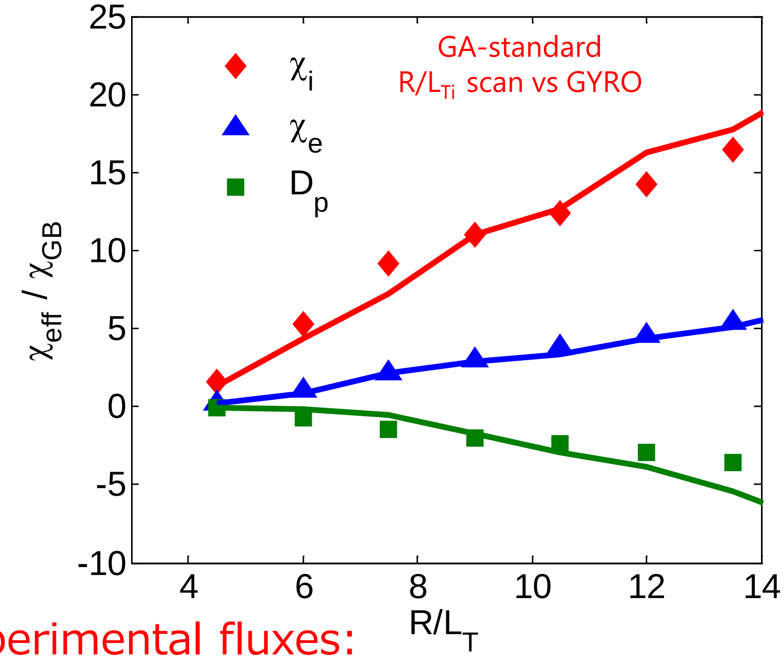
Some conseqeuences of the approximations…

- Only ITG/TEM/ETG modes are described
- Nonlinear ITG EM-stabilization effects, e.g. JC PRL 2013, PPCF 2015, Doerk 2016 PPCF, not captured. To be included in nonlinear saturation rule
- Exaggeration of α-stabilization at low $s-\alpha$, likely due to missing slab-like modes due to Gaussian eigenfunction ansatz (ongoing work O.Linder)
  Pragmatic (temporary) solution for integrated modelling: limit s-α to minimum of ~0.2 (below which GENE predicts small degree of stabilization)
- Overexaggeration of $E \times B$ stabilization at low radii (high $\frac{q}{\epsilon}$) likely due to insufficient parallel velocity gradient destabilization
  Pragmatic (temporary) solution for integrated modelling: ignore $E \times B$ stabilization for $\rho_{norm} < 0.5$

QuaLiKiz reproduces nonlinear fluxes

Scans for “GA-standard case” parameters
(numerous other scans and comparisons have also been successfully carried out)





Validation against experimental fluxes:
e.g. Tore Supra (Casati PhD 2009, Villegas PRL 2010), JET (Baiocchi NF 2015, JC, S.Breton, C. Bourdelle)

Continuous comparison of QLK to both nonlinear and experiment “part of our culture”

For transport studies, trivial parallelization of code over wavenumbers and radii

New validations, increase of code physics, and code speedup now completed (next slides)

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What's new?

Major upgrades towards pragmatic multi-channel integrated modelling

- Eigenfunction solution algorithm optimization → $\times\, 50$ speedup
- Poloidal asymmetry impact (rotation, temperature anisotropy) on heavy impurity transport [1,2]. Validated against GKW
- Impact of rotation, momentum transport [3]
- Retuning of ETG transport based on flux matched JET simulation [N. Bonanomi et al., EPS 2015]
- Coupling to JETTO-SANCO integrated modelling suite for flux driven multi-channel simulations with several ion species [4,5]
- Ongoing work with a neural network emulation of QuaLiKiz, with a factor $\times\, 10^6$ speedup for realtime capability [JC et al., NF Lett. 2015]

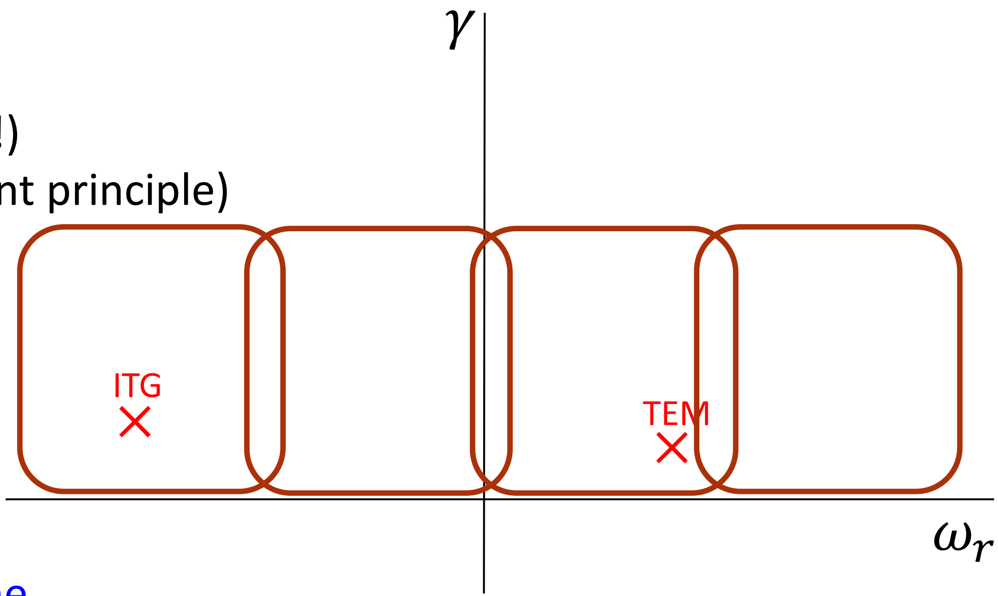
[1] C Angioni *et al.* 2012 *Phys. Plasmas* 19 122311, [2] F J Casson *et al.* 2015 *Plasma Phys. Control. Fusion* 57 014031 [3], P. Cottier *et al.,* Plasma Phys. Control. Fusion **56** (2014) 015011 [4] G. Cenacchi, A. Taroni, JETTO: A free-boundary plasma transport code, JET-IR (1988). [5] M. Romanelli *et al.*, 2003, 23rd International Toki Conference

Factor ~50 speedup achieved in last 2 years. Now ~1 CPUs for single growth rate

$D(\omega) = 0$ is a root finding problem in the complex plane

In QLK, based on Davies algorithm for finding multiple roots (Davies JCP 1986)

1. Calculate contour of $D(\omega)$ (squircles!)
2. Determine if a root is inside (argument principle)
3. If so, zero in on root (aided by Newton solver)
4. Move to next contour (goto 1)



In integrated modelling, can often start at 3 (Newton) using guess from previous timestep solution, and save significant time

- Optimization of contour search has led to a speedup of factor ~10!
- Calculation of plasma dispersion functions Z inside $D(\omega)$ now carried out by Weidman method (Gürcan JCP 2014, Weideman JNA 1994) for an additional factor ~2

Typical computation time for 1 growth rate: now ~1s
Typical computation time in stable regime: ~0.5s (no need to converge to root)
Now comparable or faster than TGLF tractability, 1 million times faster than full non-linear

Impact of heavy impurity density poloidal asymmetry now included

Poloidal asymmetries from centrifugal force and anisotropic heating (assumed bimaxwellian). They arise due to parallel force balance constraint

$$n_j(\theta,r) = n_{j,lfs}(\mathrm{r})\frac{T_{\perp j}(\theta,r)}{T_{\perp j,lfs}(r)}\exp\left[-\frac{Z_j e\Phi(\theta,r) - \frac{1}{2}m_j\Omega^2(r)\left(R_\theta(\theta,r)^2 - R_{lfs}(r)^2\right)}{T_j(r)}\right]$$

$$\frac{T_{\perp j}(\theta,r)}{T_{\perp j,lfs}(r)} = \left[\frac{T_{\perp j,lfs}(r)}{T_{\parallel j,lfs}(r)} + \left(1 - \frac{T_{\perp j,lfs}(r)}{T_{\parallel j,lfs}(r)}\right)\frac{B_{lfs}(r)}{B(\theta,r)}\right]^{-1}$$

Hinton Wong PF 1985
Casson PoP 2010
Angioni PoP 2012
Bilato NF 2014

- Equilibrium electrostatic potential Φ calculated numerically via θ-dependent quasineutrality
- 2D density and density gradients adds new terms to quasilinear flux equation
- High Z and high A impurities can be strongly impacted, even for low main species Mach number
- QuaLiKiz now can include arbitrary number of ion species (active or tracer)

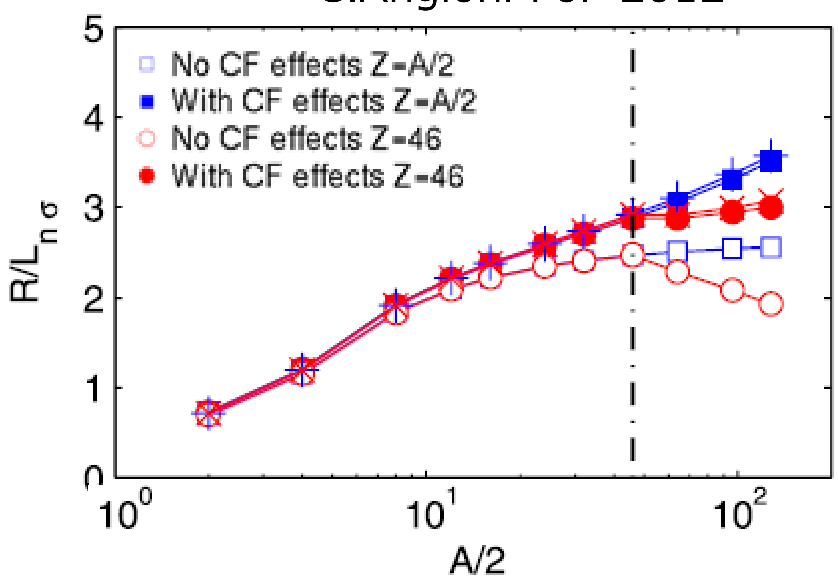
Successful first comparison between GKW QL and QualiKiz heavy impurity

Test zero-flux R/Ln versus ITG test case published in Angioni POP 2012

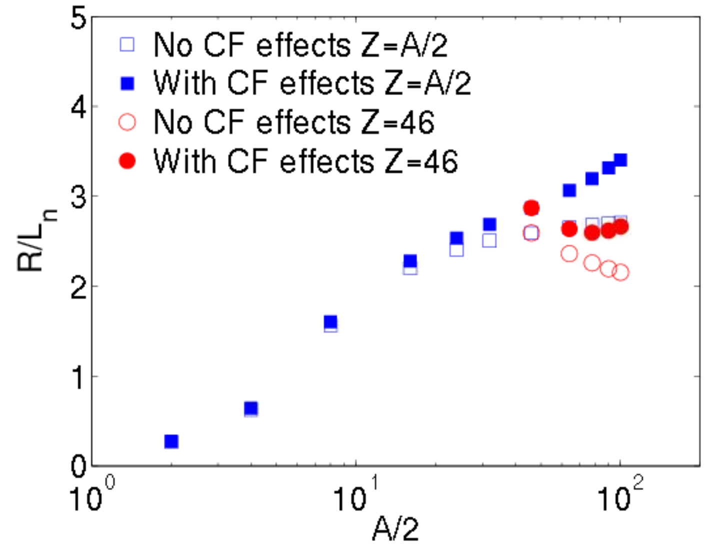
$$k_y\rho_s = 0.3, \mathrm{q} = 1.4, \hat{s} = 0.8, \frac{R}{L_{Ti}} = 9, \frac{R}{L_{Te}} = 6, \frac{R}{L_n} = 2, \epsilon = \frac{1}{6}, \mathrm{M} = 0.1, \frac{\mathrm{R}}{\mathrm{L_u}} = 5$$

Effective centrifugal thermodiffusion, rotodiffusion, and convective pinch terms calculated in QuaLiKiz very similarly (but not identical to) Angioni PoP 2012

C.Angioni PoP 2012



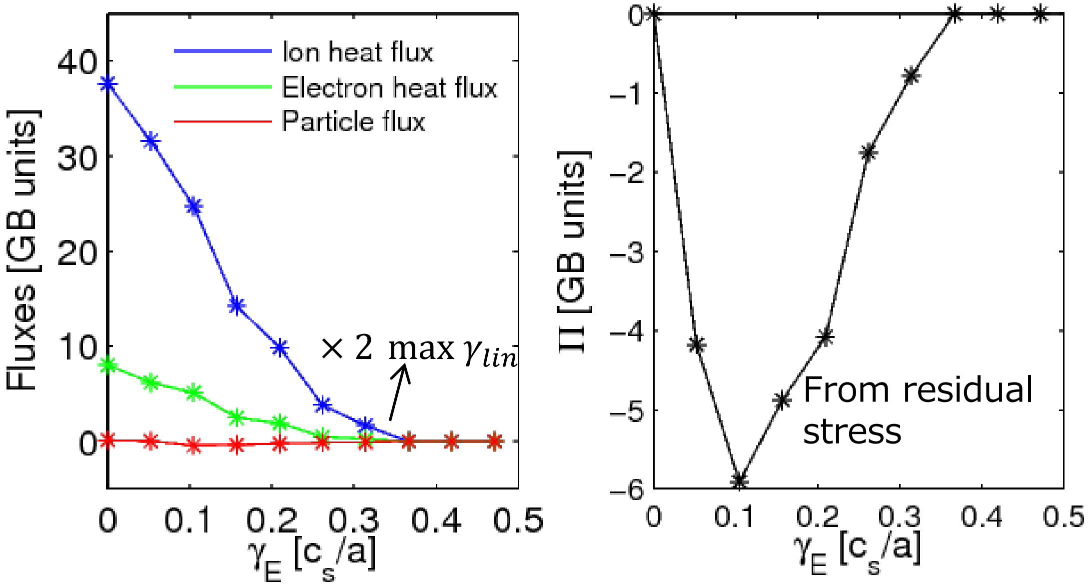
QuaLiKiz



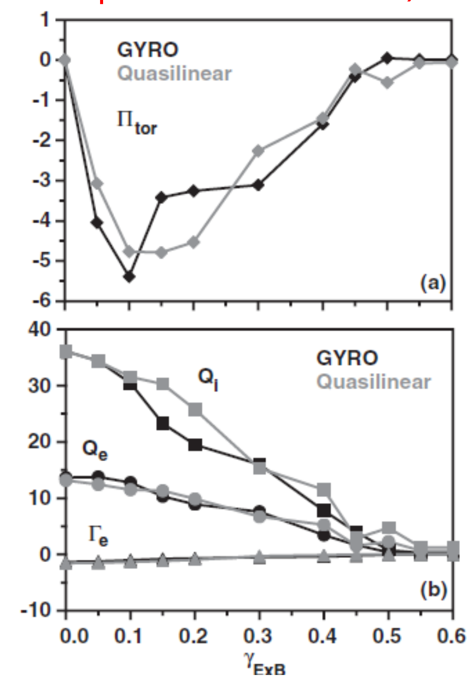
- Correspondence generally within ~10% for most cases
- 1 second of computation time for QuaLiKiz to produce this plot!

Validation of ExB suppresion and momentum transport

GA-STD γ_E scan (with collisions)

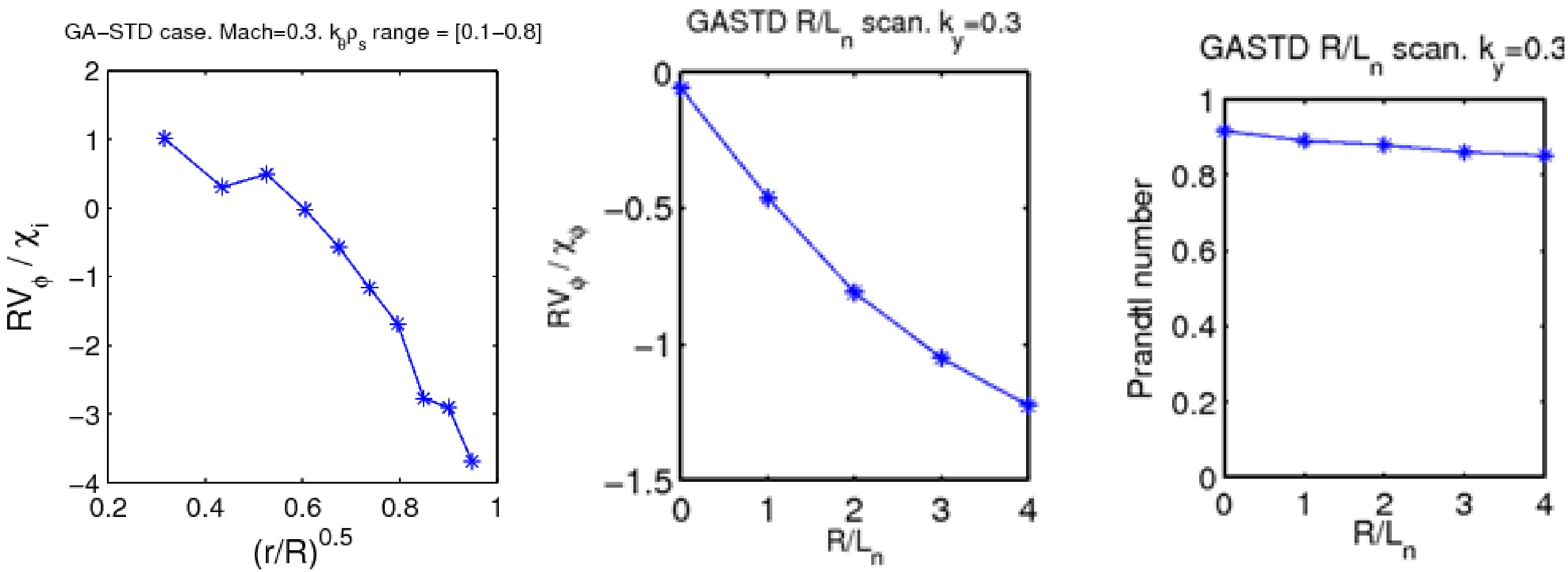


Staebler PRL 2013 (GYRO and TGLF spectral shift model)



- GA-STD γ_E scans (Cottier PPCF 2014). Agrees with GYRO+TGLF
- The solver calculates the shifted eigenfunction due to u, u′, γ_E. Symmetry breaking in dispersion relation and quasilinear flux integrals

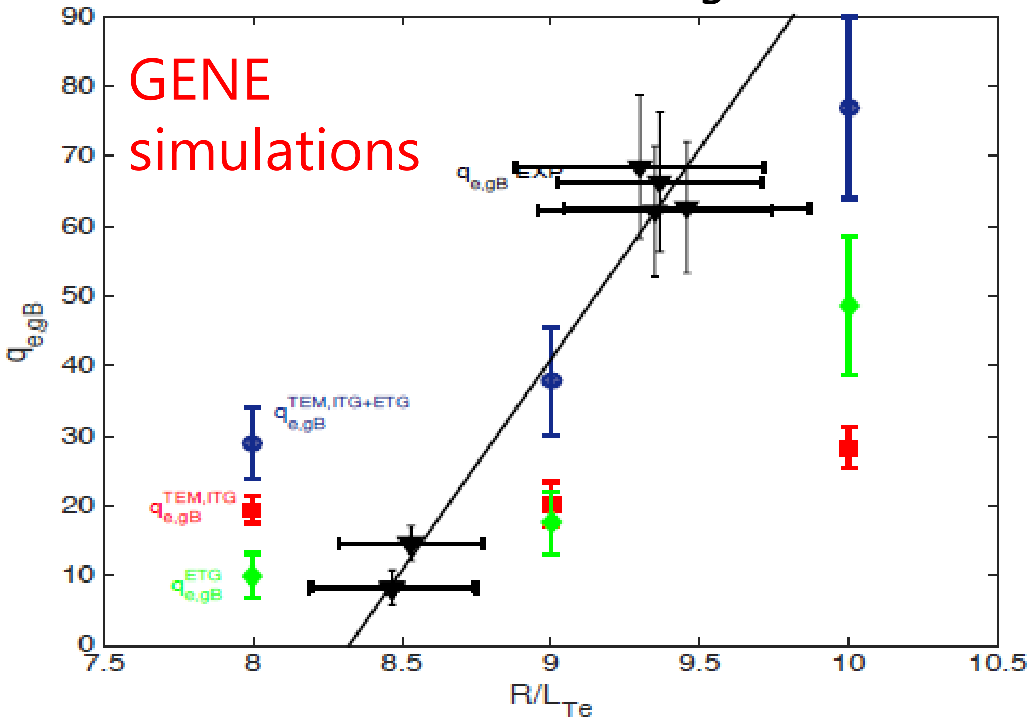
QuaLiKiz reproduces increasing momentum pinch with trapped electron drive



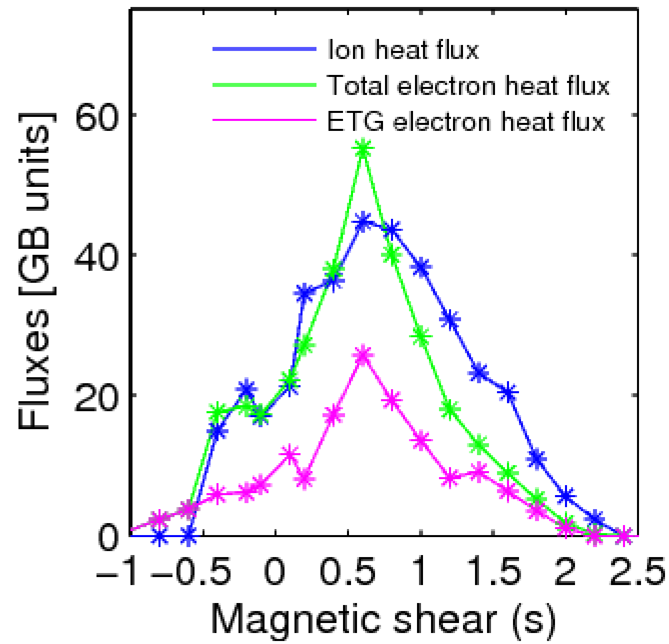
- QuaLiKiz reproduces increasing momentum pinch with trapped electron drive
  Seen with either increasing R/Ln or increasing ϵ
- Pr ~ 1 in pure u' scan with no strong dependence on R/Ln
- Consistent with theory and GKW simulations (review in Peeters et al 2011)

ETG contribution in QuaLiKiz fluxes based on recent work on JET

From Bonanomi et al. EPS 2015
ICRH heated JET discharge 78834



QuaLiKiz GA-STD s-scan
with new ETG contribution



- GENE single-scale NL simulation with γ_E to break apart streamers and avoid box effects. ~50% of electron power balance in agreement with observation. Used to tune nonlinear saturation rule in QuaLiKiz single scale ETG
- Impact shown on GASTD case magnetic shear scan. Up to 50% of q_e in some cases

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QuaLiKiz ready for integrated modelling

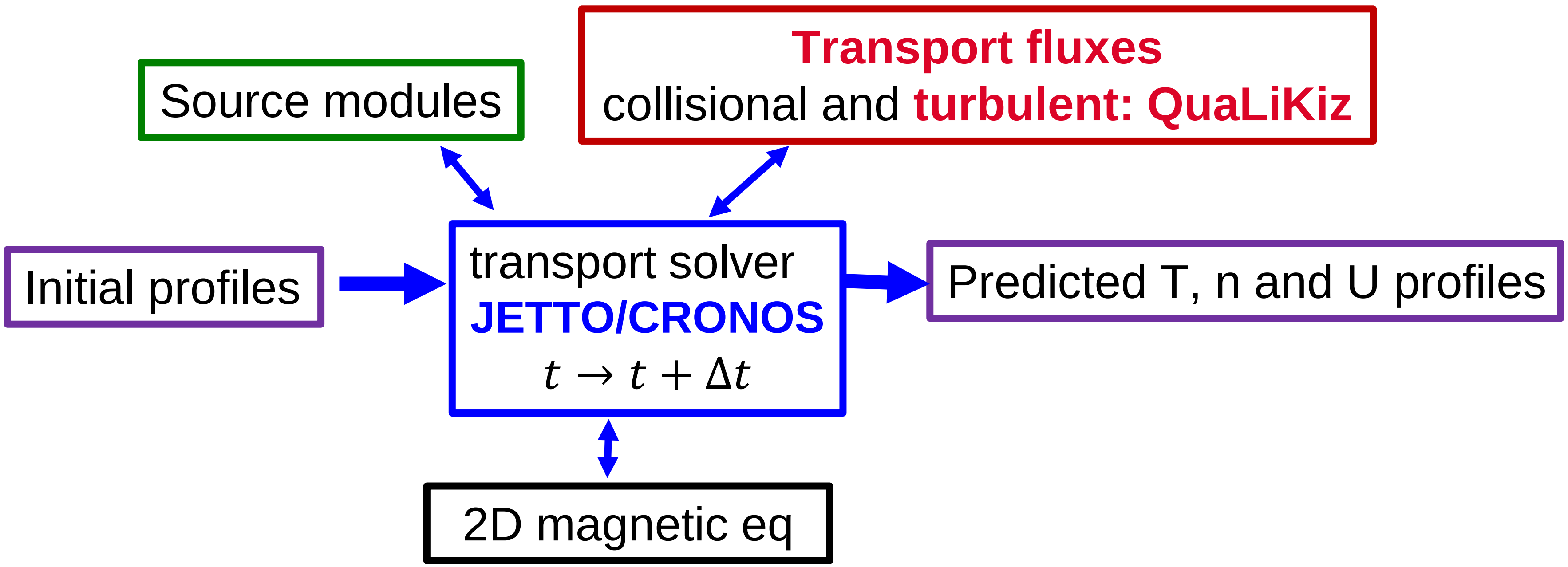
QuaLiKiz turbulent fluxes = Quasilinear + other approximations

$t_{turb.fluxes}$~$20s$ for a profile i.e. 20 radial points, 10 $k_\theta \rho_s$, 10 CPUs

$t_{turb.fluxes}$~$2-5\ s$ when starting from previous, similar, solution

- reproduces well nonlinear gyrokinetic fluxes over wide range of parameters in ~10^6 less computing time

→ ready for integrated modeling



Extensive coupling work to JETTO-SANCO

JETTO – flux driven transport solver with sources and equilibrium

SANCO – impurity density and charge state evolution, radiation

- Includes Pereverzev and G. Corrigan numerical treatment for stiff transport
- Neoclassical transport from NCLASS or NEO

1s of JET plasma takes ~20h walltime with QuaLiKiz on 16 CPUs (2.33GHz)
(Note: this is with rotation. Without rotation, around $\times 4$ quicker due to symmetry in 2D integration)

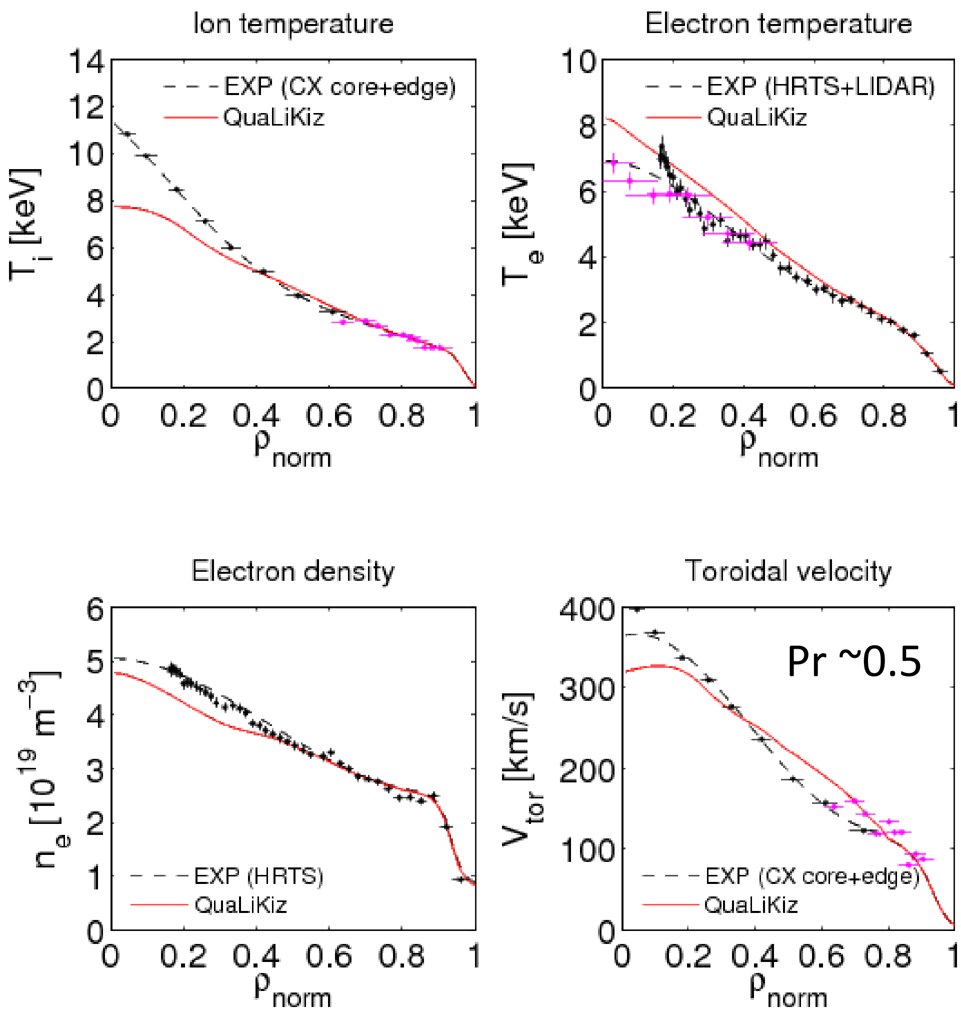
Extensive testing done on well diagnosed and studied hybrid scenario 75225 and baseline scenario 87412

First QuaLiKiz integrated modelling simulations with impact of rotation on turbulence, multiple ions, and momentum transport

Main result: JETTO-SANCO integrated modelling

Agreement excellent in ALL channels for ρ>0.5

First ever 4-channel flux driven QuaLiKiz simulation. ~100 CPUh



JET 75225 (C-wall hybrid scenario)
Time window from 6-7s

C impurity in SANCO → D and C modelled separately

Boundary condition at $\rho = 0.8$

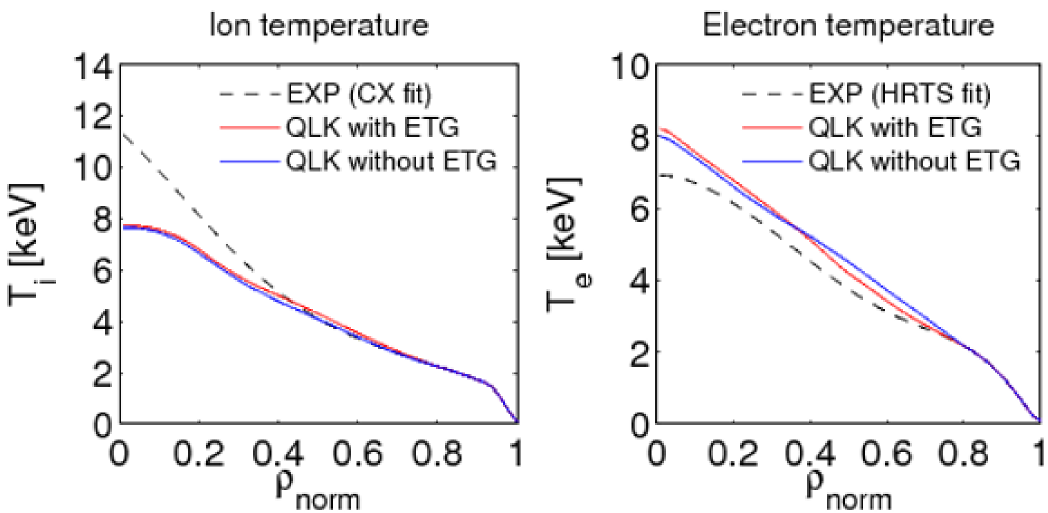
Includes rotation ($\rho > 0.5$) and momentum transport!

Agreement excellent in all channels for $\rho > 0.5$

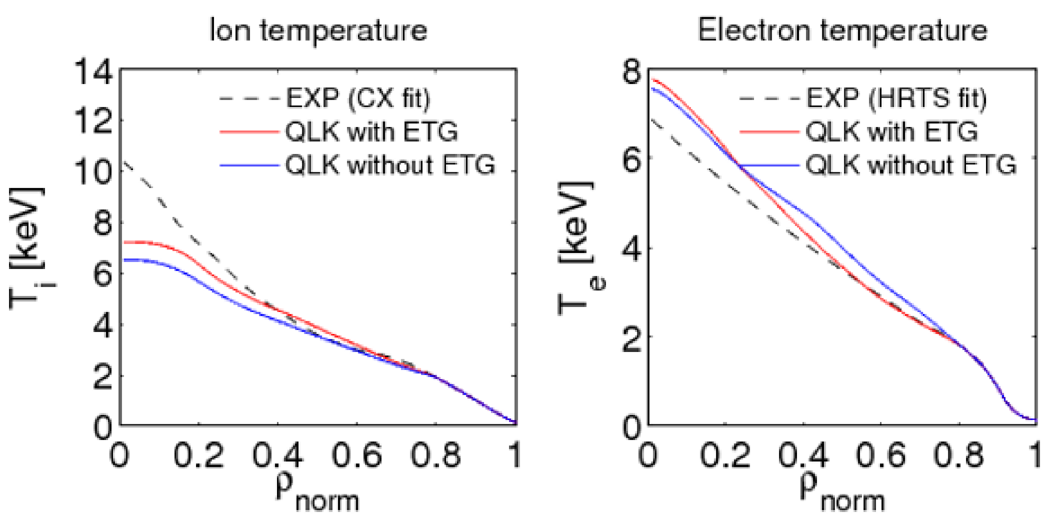
For $\rho < 0.5$, Ti underprediction due to lack of EM effects in QLK

Sensitivity to ETG model in JET hybrid scenario integrated modelling

Comparison with and without ETG model



Original fit and boundary conditions

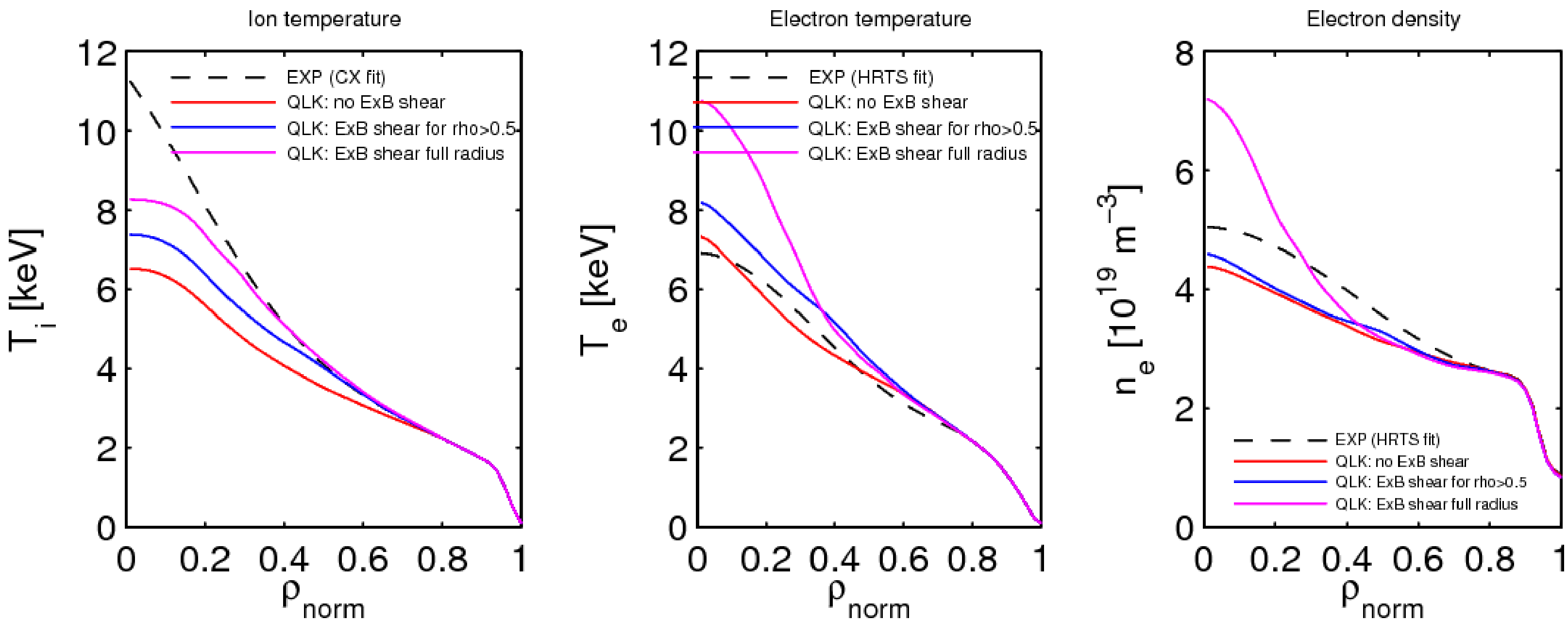


Fit with reduced T_e, T_i boundary conditions at $\rho = 0.8$ by ~20%

ETG scales can be important for agreement, but sensitive to e.g. boundary conditions

QuaLiKiz ExB shearing model leads to agreement at $\rho > 0.5$

Sensitivity to rotation settings

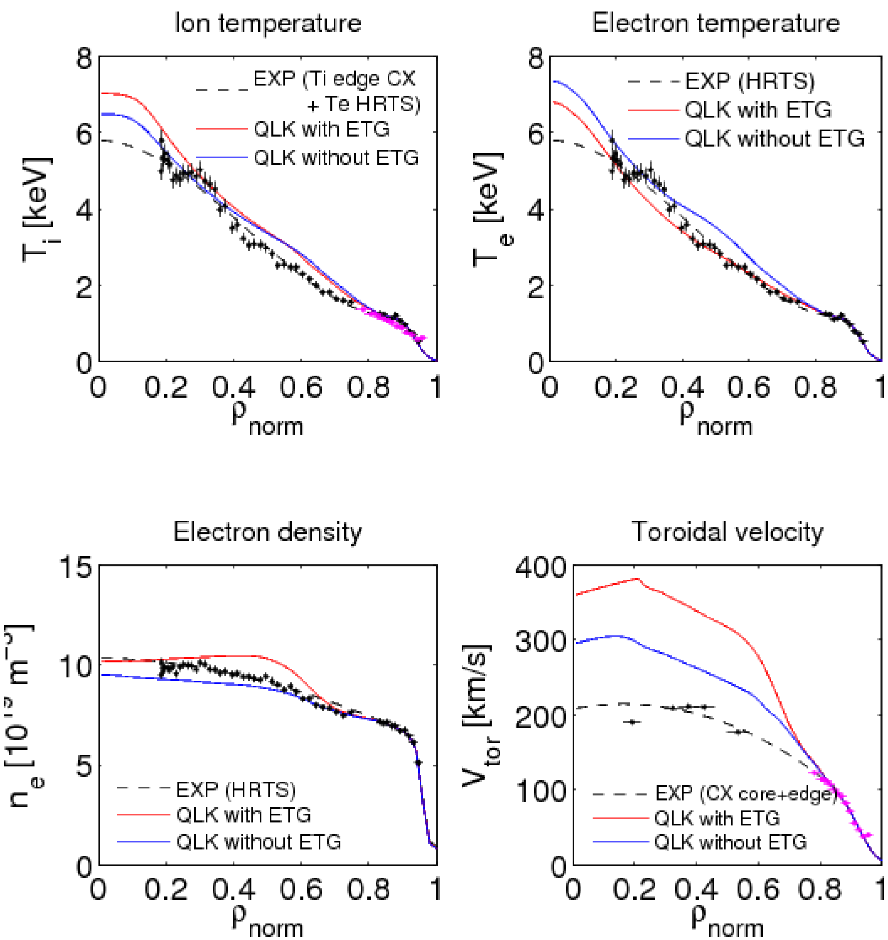


- Reminder: ExB shearing not kept for $\rho < 0.5$ in integrated modelling
- Including ExB shear at $\rho > 0.5$ important for agreement
- T_i "Agreement" when including ExB shear at entire radius is erroneous. Also leads to n_e, T_e overprediction since completely stable for $\rho < 0.4$
- QLK likely underestimates PVG destabilization (under investigation)

JETTO-QLK modelling of a JET baseline scenario

ILW baseline scenario
JET 87412 (3.5MA/3.35T)

Comparison with and without ETG-scales
Time window averaged between 10-10.5s

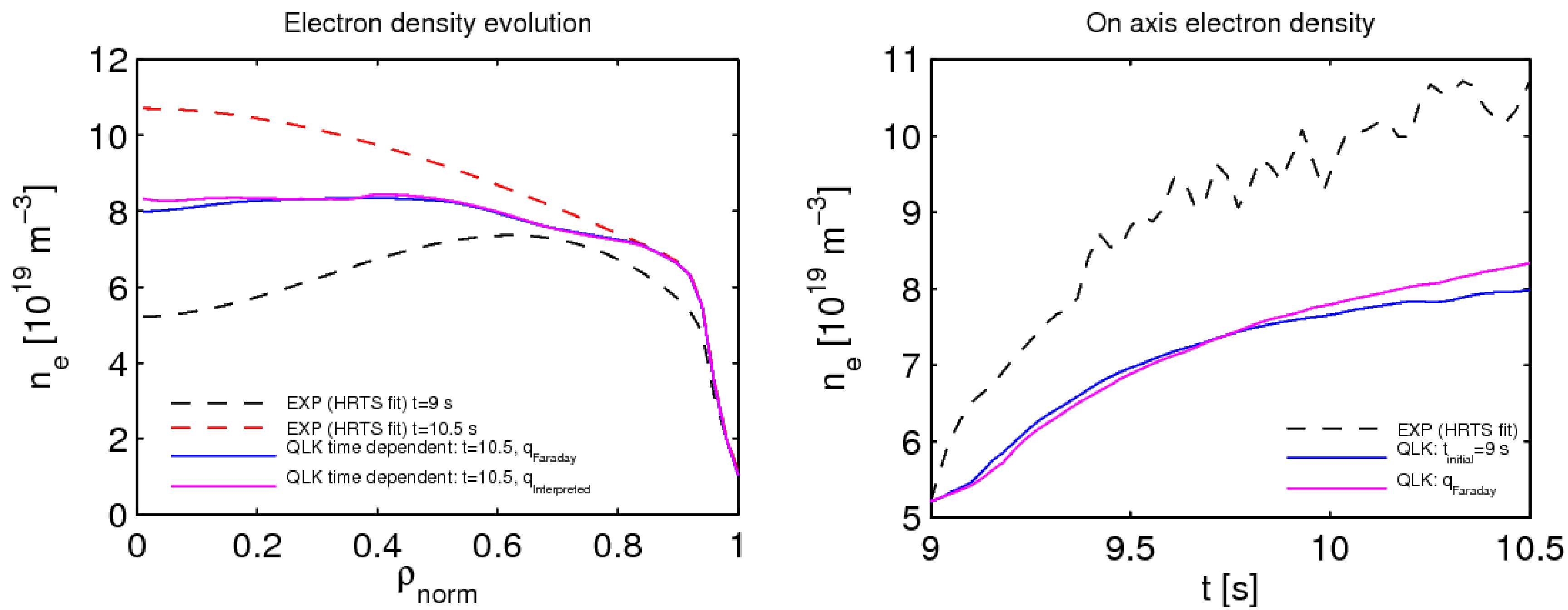


Good agreement in
All channels apart from V_{tor}

- Boundary condition at $\rho = 0.85$
- Stable for $\rho < 0.2$. No sawtooth model
- Assuming core measurements $T_i = T_e$ due to poor core CX
- NTV torque due to NTMs flatten profile?
- Interesting interplay between momentum transport and profiles obtained without ETG. Under investigation

Buildup of density following LH transition partially recovered by QuaLiKiz

Dynamic simulation of density buildup following LH transition



- Anomaly in early phase 9-9.5s. General trend reasonably captured for t>9.5s
- Additional examples ongoing, with even more positive results (S. Breton, C. Bourdelle, ongoing work)
- Weak dependence here on q-profile assumption (polarimetry vs modelled)

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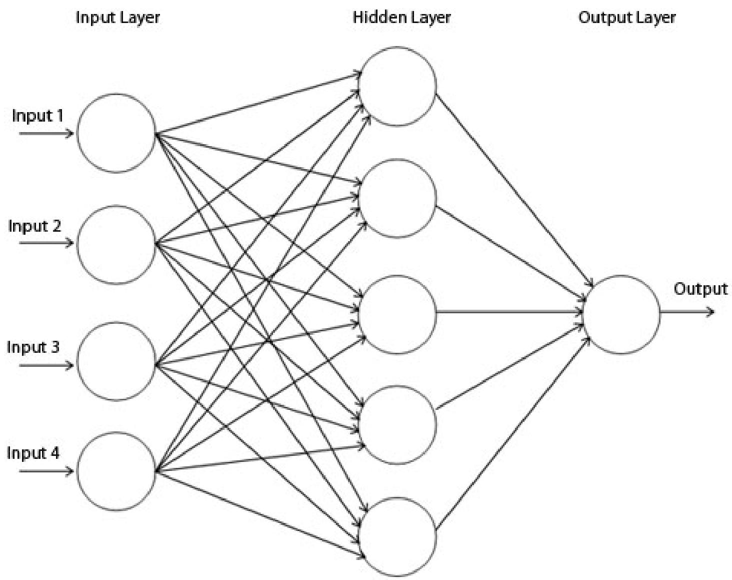
Neural network QuaLiKiz – a realtime first-principle-based transport model



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

Linear superposition into nonlinear functions, e.g. tanh, sigmoid

Outputs: e.g. ion heat flux, pedestal height

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

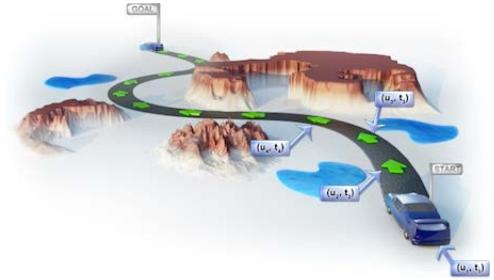
With, e.g. $g(x) = \dfrac{2}{1+e^{-x}} - 1$

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

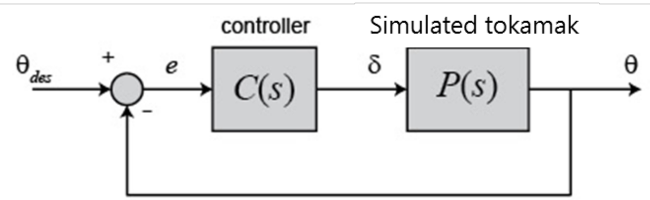
- Optimal weights found by optimization based on 'training set' of known mapping
- Can be used as a nonlinear regression technique to emulate transport models
- Trained network output in <ms, orders of magnitude less than original calc. circumvents conflicting constraints of model accuracy and tractability
- Provides an analytical formula with analytical derivatives. Critical for trajectory optimization and implicit timestep solvers

Neural network technique opens up wide applications for IOS prediction and control

“Very fast” tokamak simulator

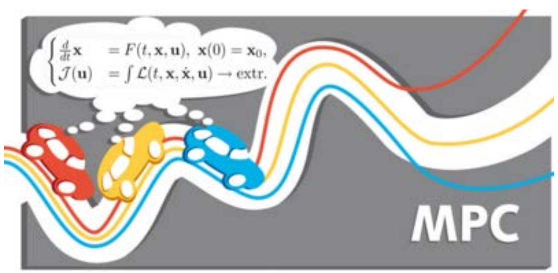


- Offline trajectory optimization
- Controller design
- Controller validation



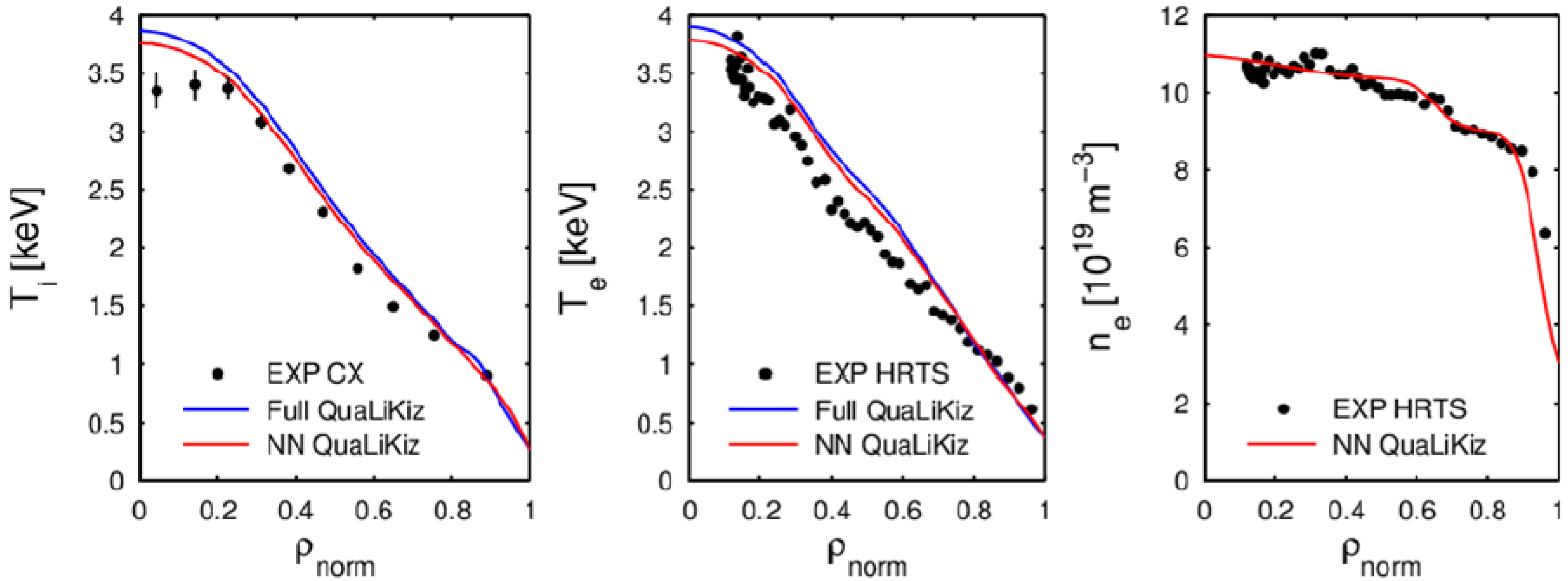
Realtime tokamak simulator

- Discharge supervision and monitoring (e.g. disruption mitigation)
- Online trajectory optimization faster-than-real-time (model-based predictive control)



Neural network QuaLiKiz: Ti, Te and ne

CRONOS/QLKANN simulation of flat top in JET 73342 standard H-mode.
Boundary condition at $\rho = 0.88$



- QuaLiKiz kinetic electron ITG database constructed. Dense parameter space variation of R/LTi, Ti/Te, s, q. $O(10^4)$ QuaLiKiz runs used for neural network training. Neural network successfully reproduces QuaLiKiz results $\times 10^6$ faster!
- Already works surprisingly well on JET ITG dominated case in flux driven modelling
- In progress: Dense 10D input space population within ranges set by experiments

Summary and outlook

- Extensive speedup and new physics greatly extends applicability of QuaLiKiz gyrokinetic quasilinear turbulent code
- First multi-channel $(T_e, T_i, n_e, n_{imp}, v_{tor})$ QuaLiKiz simulations of JET discharges with encouraging validation in JETTO-SANCO

Outlook

- Ongoing work on W-transport in JET in conjunction with NEO for neoclassical transport (S. Breton, F. Casson)
- Ongoing work on ITER modelling (B. Baiocchi, this conference)
- LOC-SOC transitions on JET (C. Bourdelle)
- Ongoing neural network emulation of QuaLiKiz for realtime capability

Sketch of QuaLiKiz model construction (3)

Dispersion relation: passing, trapped, trapped electrons

$$D(\omega) = \sum_s \int drd\theta d\lambda d\epsilon \, \frac{n_s e_s^2}{T_s}\left(1 - \frac{\omega_k - n\omega_s^*}{\omega_k - [k_\parallel v_\parallel, 0] + i\nu - n\omega_{sD}} J_0^2(\mathrm{k}_\perp[\rho_s, \delta_s])|\delta\phi(r,\theta)|^2\right) = 0$$

Integrations

- Energy: plasma dispersion function (though not for trapped electrons)
- Pitch angle: Approximated $\langle k_\parallel v_\parallel \rangle, \langle \omega_d \rangle$ for passing
- θ, bounce average for trapped species (elliptic integrals in low r/R ordering)
- r, trivial for trapped species (only over known eigenfunction)

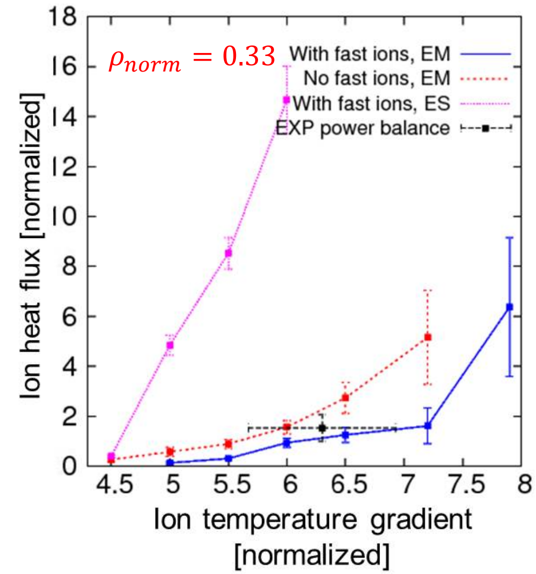
→ 1D adaptive numerical integration for trapped ions (pitch angle)

2D adaptive numerical integration for passing ions (r, θ), and
for trapped electrons (pitch angle, energy): bottleneck in calculation

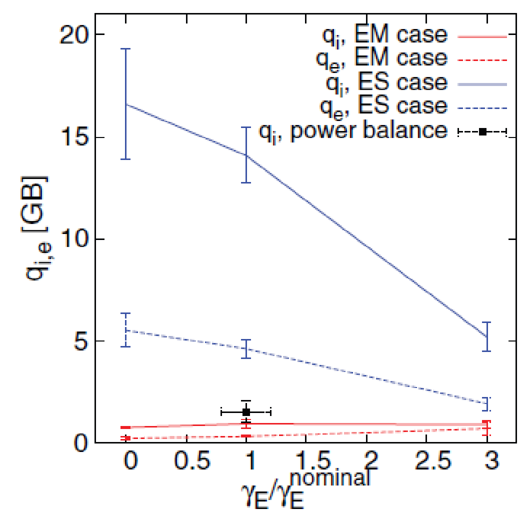
Caveats: specific challenges for QuaLiKiz in hybrid scenarios

- Nonlinearly enhanced EM-stabilization at $\rho < 0.5$
- QuaLiKiz is electrostatic, and this effect not included in QuaLiKiz saturation rule

GENE NL simulations of 75225



- GENE and GYRO simulations show a negligible impact of rotation on this case for $\rho < 0.5$ (R. Bravenec, submitted to PPCF, and JC PPCF 2015)
- Occurs when ITG is in EM-stabilized regime
- Also in ILW hybrids (H. Doerk, submitted to PPCF)

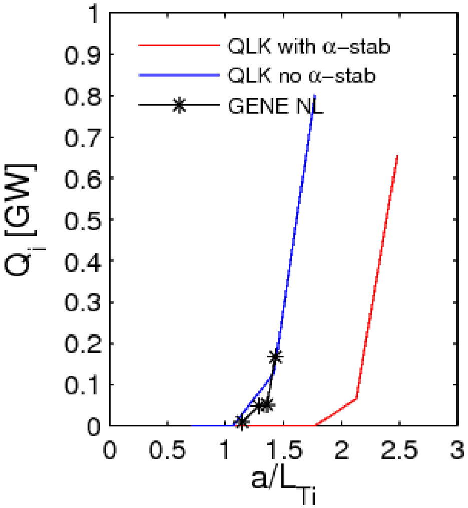


Caveats: specific challenges for QuaLiKiz in hybrid scenarios

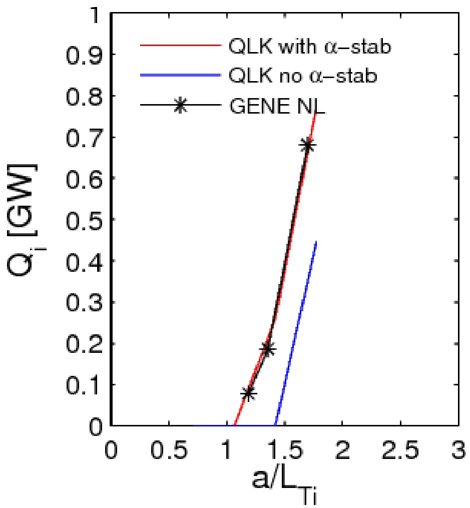
α-stabilization at low magnetic shear (as in hybrids inner half-radii) is known to be exaggerated in QuaLiKiz, likely due to ballooned eigenfunction ansatz

QuaLiKiz-GENE comparison for the DEMO1 scenario. (with T. Goerler)

$\rho = 0.35,\ s = 0.24$



$\rho = 0.53,\ s = 0.94$



Threshold and stiffness agreement excellent for moderate magnetic shear (where it is actually destabilization).

At low magnetic shear, agreement excellent when not including α-stabilization in QuaLiKiz

- Thus, based on these GENE comparisons and simulations: we set α-stabilization, and impact of rotation on the eigenvalues, only for $\rho > 0.5$. Linear GENE scans show “flat” response of growth rates to increasing α at low $s - \alpha$ (O. Linder)
- Baselines should be easier to model with QuaLiKiz (lower alpha, more electrostatic, sawteeth in inner core)