Local, flux-driven, multi-channel simulations with the quasilinear gyrokinetic tokamak transport model QuaLiKiz

J. Citrin[1,2], C. Bourdelle[2], F. Casson[3], C. Angioni[4], S. Breton[2], F. Felici[5], X. Garbet[2], O. Gürcan[6], L. Garzotti[3], F. Koechl[7], F. Imbeaux[2], O. Linder[5], J. Redondo[2], P. Strand[8], G. Szepesi[9,3] and JET Contributors*
EUROfusion Consortium, JET, Culham Science Centre, Abingdon, OX14 3DB, UK

[1] *FOM Institute DIFFER, PO Box 6336, 5600 HH, Eindhoven, The Netherlands*
[2]*CEA, IRFM, F-13108 Saint Paul Lez Durance, France*
[3]*CCFE, Culham Science Centre, Abingdon, Oxon, OX14 3DB, UK*
[4]*Max Planck Institute for Plasma Physics, Boltzmannstr. 2, 85748 Garching, Germany*
[5]*Eindhoven University of Technology, The Netherlands*
[6] *LPP, Ecole Polytechnique, CNRS, 91128 Palaiseau, France*
[7] *ÖAW/ATI, Atominstitut, TU Wien, 1020 Vienna, Austria*
[8] *Department of Earth and Space Sciences, Chalmers University of Technology, SE-412 96 Göteborg, Sweden*
[9] *Istituto di Fisica del Plasma CNR, 20125 Milano, Italy*
**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

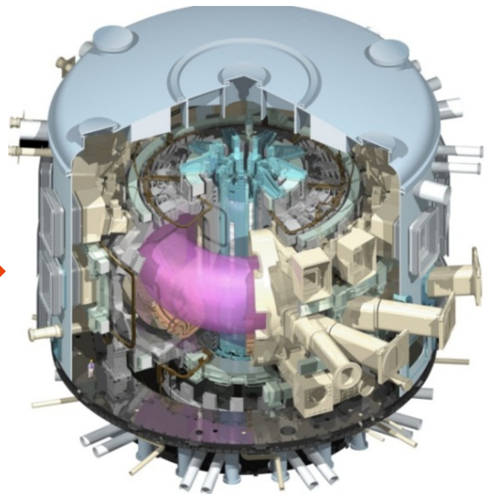
Magnetic equilibrium

Heating

MHD stability

Turbulence

Plasma-wall-interaction



Fusion power

Heat exhaust

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

QuaLiKiz is a fast code for standalone or integrated modelling turbulent fluxes

Quasilinear gyrokinetic model for transport fluxes (C.Bourdelle POP 2007, PPCF 2016)

- Saturation rule normalized to single ion-scale and electron-scale nonlinear simulations. Correction at low magnetic shear (Citrin PoP 2012)
- Particle, heat, impurity, and momentum fluxes from ITG, TEM, ETG

Major approximations

- Electrostatic only
- s-α geometry with small inverse-aspect ratio expansion
- Eigenfunctions limited to ballooned structures. Reproduces well ITG-ETG, underestimation of transport in TEM k-range

Nevertheless, wide operational regime of validity. And further improvements can still be made

Brief overview of QuaLiKiz model (1): simplified GK dispersion relation

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

Linearized Vlasov (electrostatic)

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

Weak form for quasineutrality

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)

Brief overview of QuaLiKiz model (2): saturation rule for nonlinear fluxes

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 - 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"

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

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

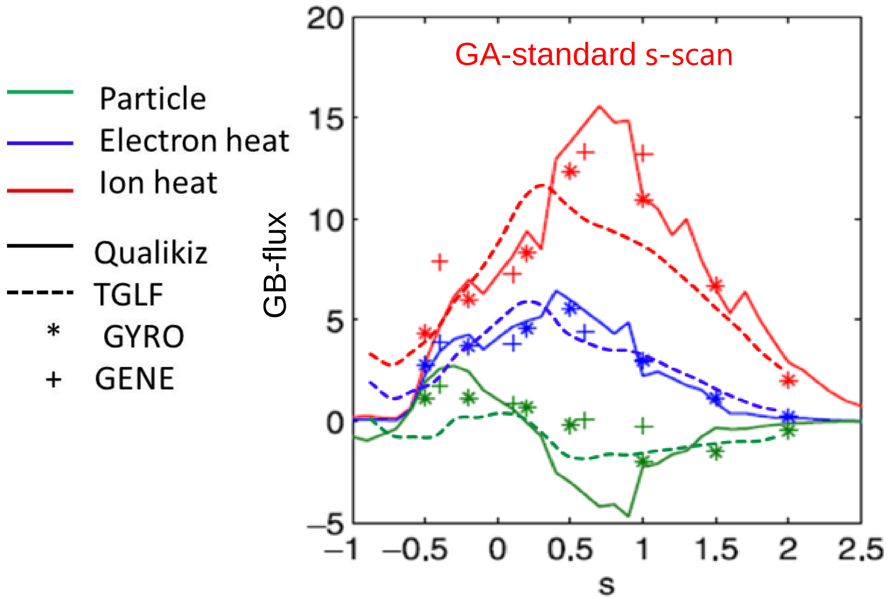
$$|\delta\phi_k|^2 = C S_k \max\left(\frac{\gamma_k}{k_\perp^2}\right)$$

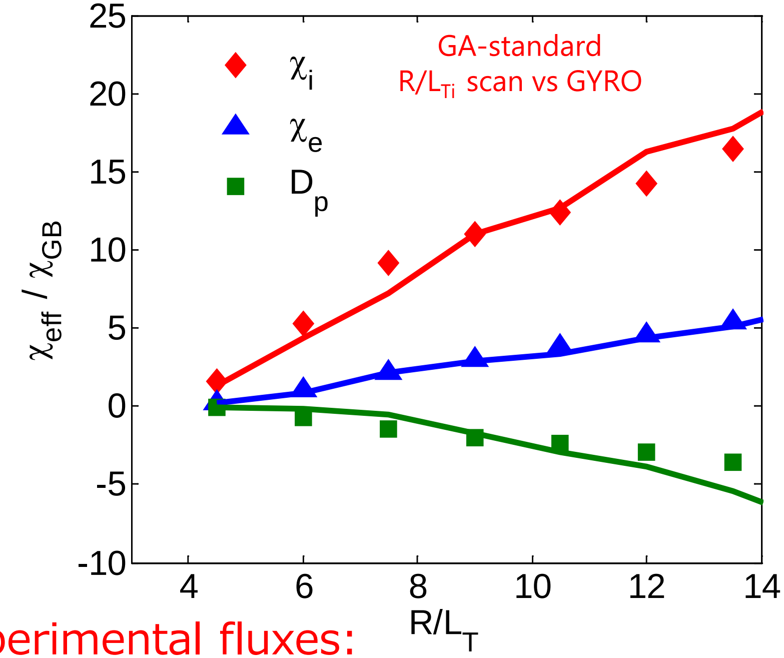
C is scalar factor set by matching ion heat flux in single NL simulation (for ion and electron scales separately)

$< k_\perp^2 >= k_\theta^2(1+s^2 < \theta^2 >)$ + finite k_x corrections at low magnetic shear

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 EPS 2016)

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)

What's new?

Major upgrades towards pragmatic multi-channel integrated modelling

- Eigenfunction solution algorithm optimization → $\times 50$ speedup
- Arbitrary number of ion species
- 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]

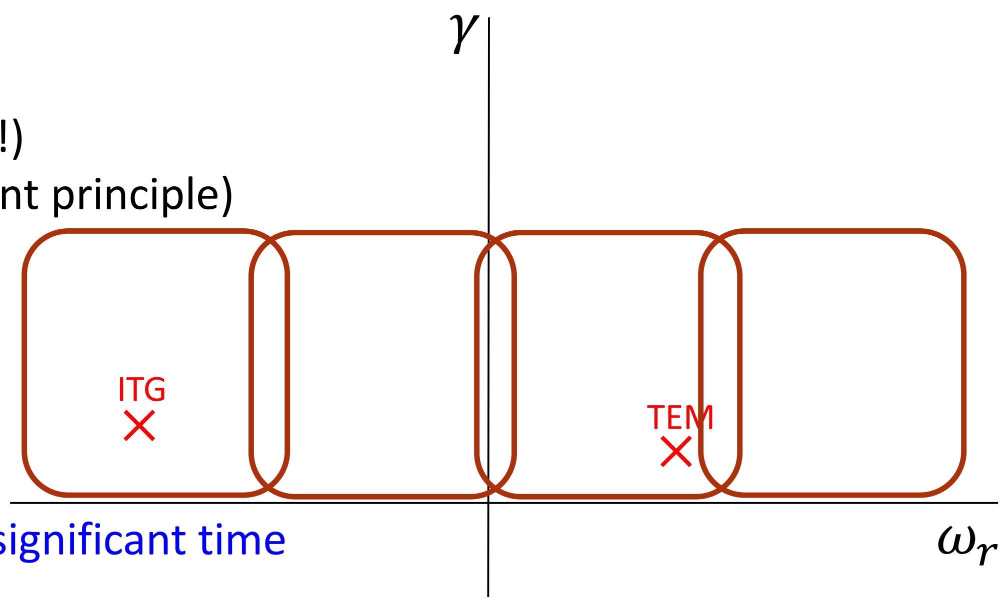
[1] C Angioni *et al.* 2012 *Phys. Plasmas* 19 122311, [2] F J Casson *et al.* 2015 *Plasma Phys. Control. Fusion* 57 014031 [3], P. Cottier *et al.,* Plasma Phys. Control. Fusion **56** (2014) 015011 [4] G. Cenacchi, A. Taroni, JETTO: A free-boundary plasma transport code, JET-IR (1988). [5] M. Romanelli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

Factor ~20-50 speedup achieved in last 2 years. Now comparable to TGLF

$D(\omega) = 0$ 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 Newton from previous solution and save significant time

- Optimization of contour search has led to a speedup of factor ~10!
- In addition, 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: ~0.3s (no need to converge to root)

Now comparable with 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)

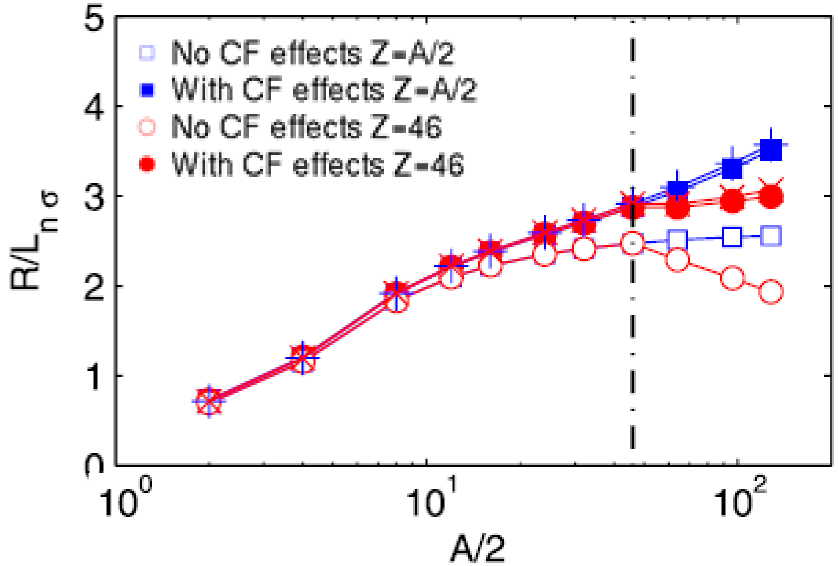
Successful first comparison between GKW QL and QualiKiz heavy impurity

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

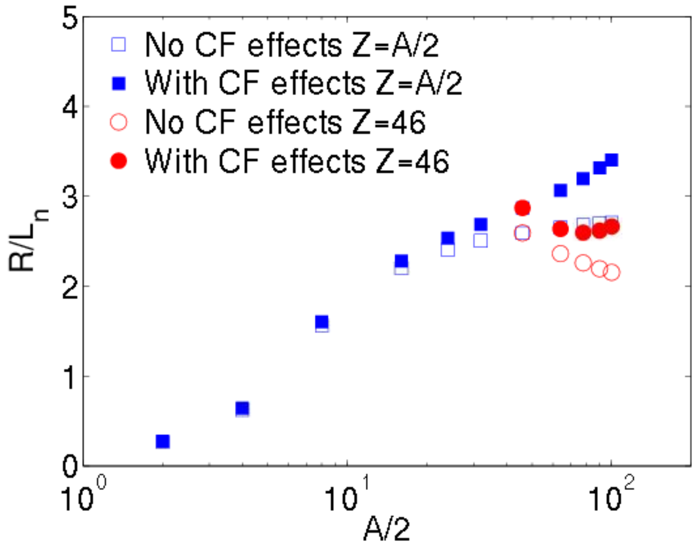
$$k_y\rho_s = 0.3, \mathrm{q} = 1.4, \hat{s} = 0.8, \frac{R}{L_{Ti}} = 9, \frac{R}{L_{Te}} = 6, \frac{R}{L_n} = 2, \epsilon = \frac{1}{6}, \mathrm{M} = 0.1, \frac{\mathrm{R}}{\mathrm{L_u}} = 5$$

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

C.Angioni PoP 2012



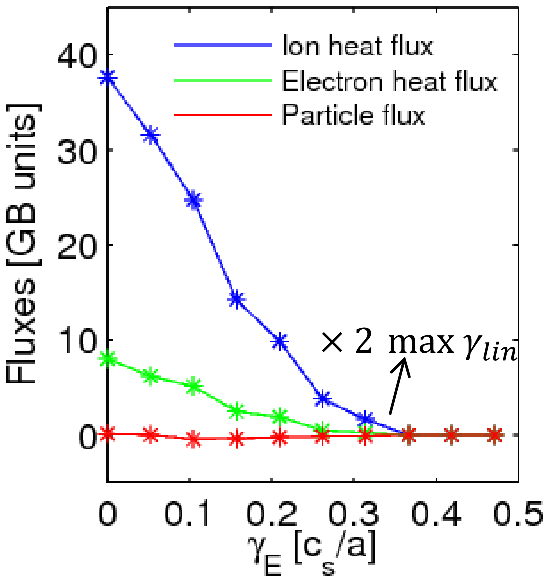
QuaLiKiz

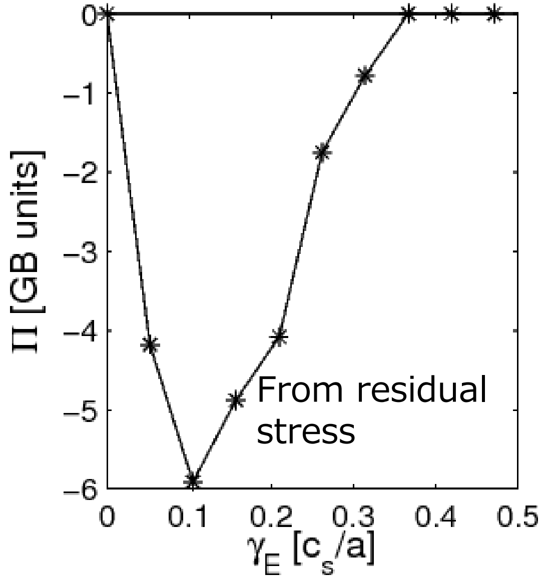


- Correspondence generally within ~10% for most cases
- 1 second of computation time for QuaLiKiz to produce this plot!

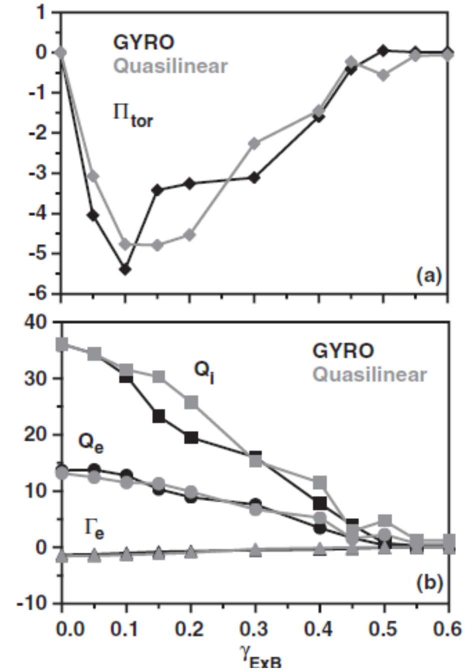
Validation of ExB suppresion and momentum transport

GA-STD γ_E scan (with collisions)



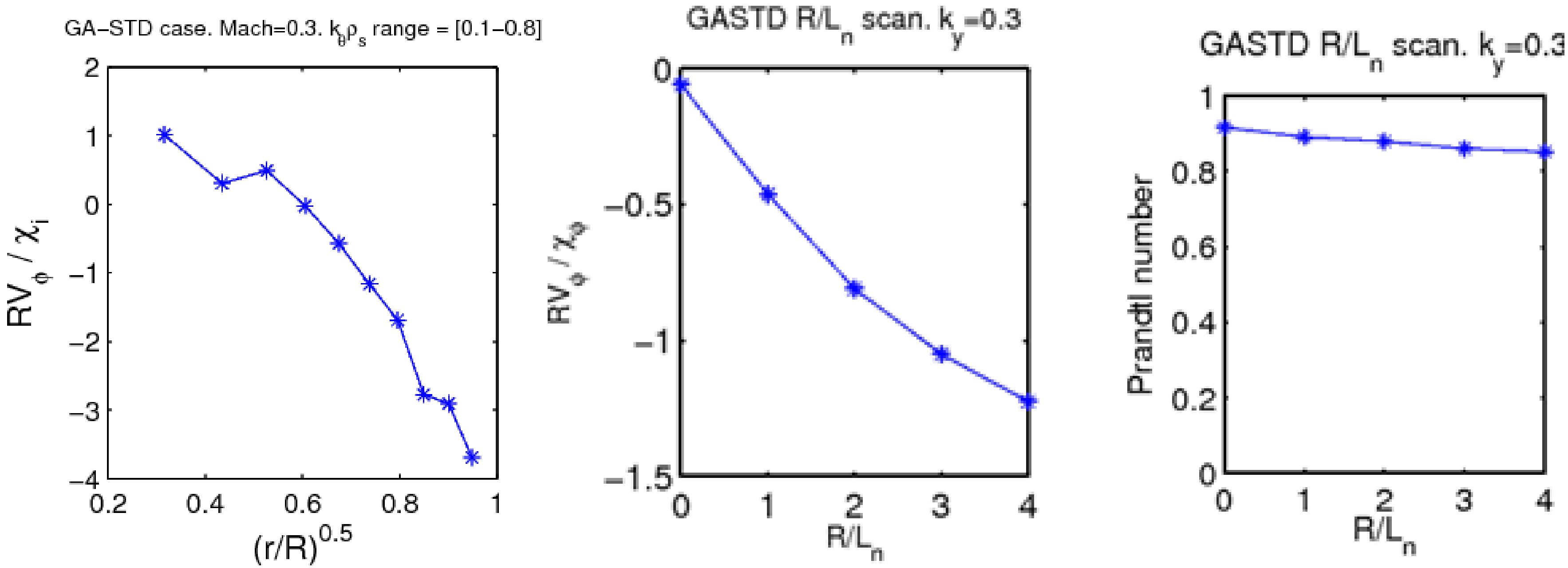


Staebler PRL 2013 (GYRO and TGLF spectral shift model)



- GA-STD γ_E scans reproduced (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

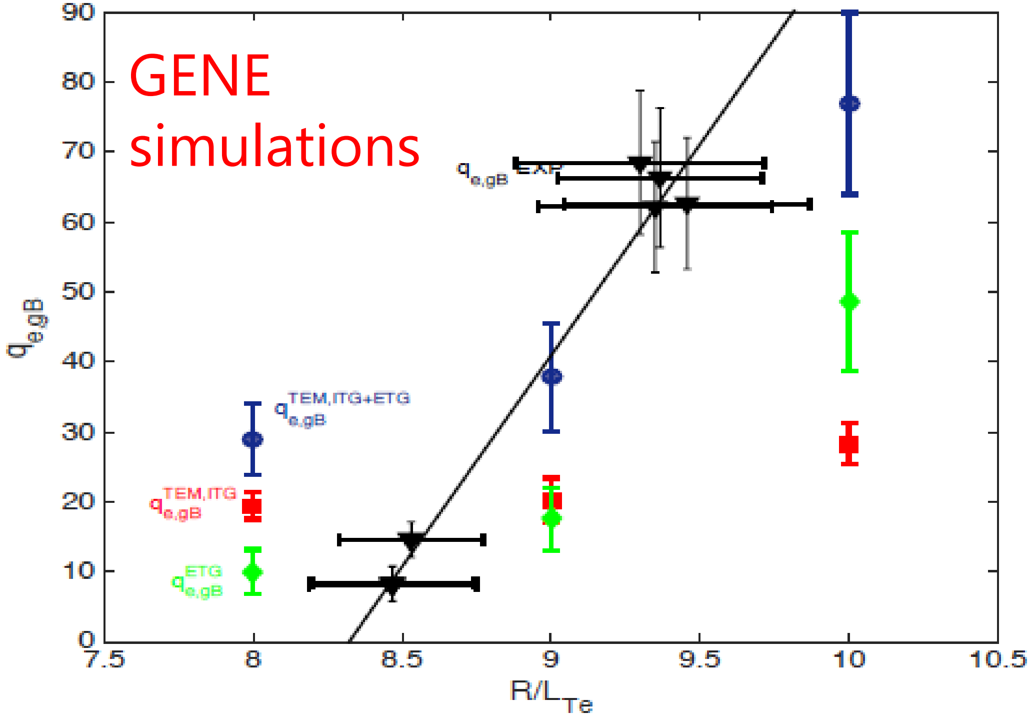
QuaLiKiz reproduces increasing momentum pinch with trapped electron drive



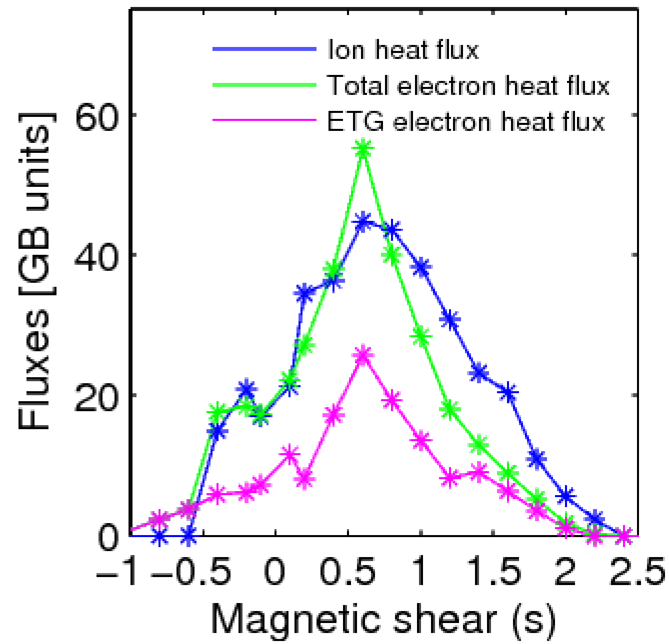
- QuaLiKiz reproduces increasing momentum pinch with trapped electron drive
  Seen with either increasing R/Ln or increasing ϵ
- Pr ~ 1 in pure u' scan with no strong dependence on R/Ln
- Consistent with theory and GKW simulations (review in Peeters et al 2011)

ETG contribution in QuaLiKiz fluxes based on recent work on JET

From Bonanomi et al. 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

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

- Coupling carried out through Par Strand's "Transport Code Interface" (TCI). Facilitates future coupling to other integrated modelling suites

1s of JET plasma takes ~5-15h walltime with QuaLiKiz on 16 CPUs (2.33GHz)

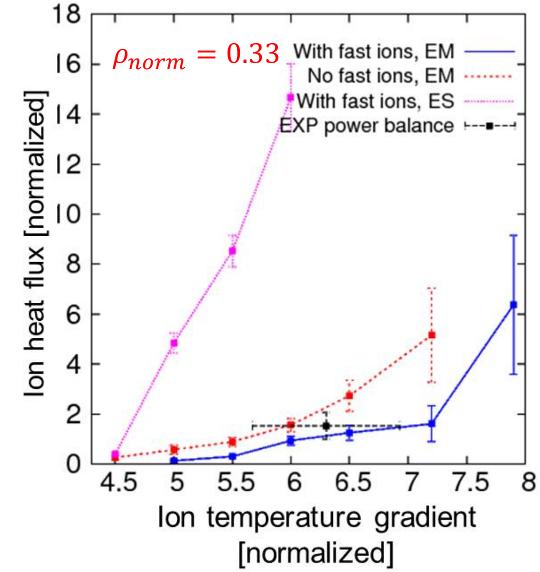
Extensive testing done on well diagnosed and studied hybrid scenario 75225

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

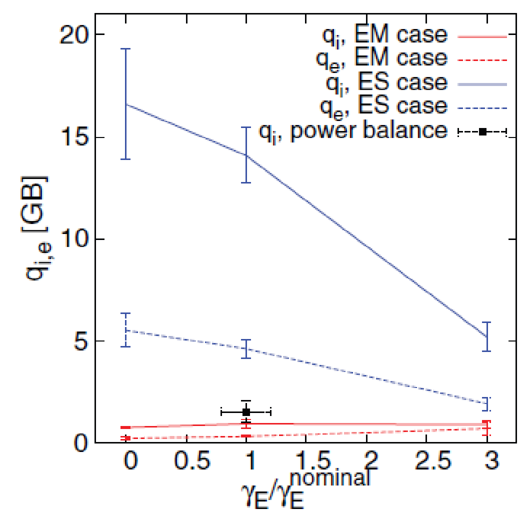
Specific challenges for QuaLiKiz in hybrid scenarios

- 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, in preparation. and JC PPCF 2015)
- Occurs when ITG is in EM-stabilized regime
- Also in ILW hybrids (H. Doerk, submitted to PPCF)

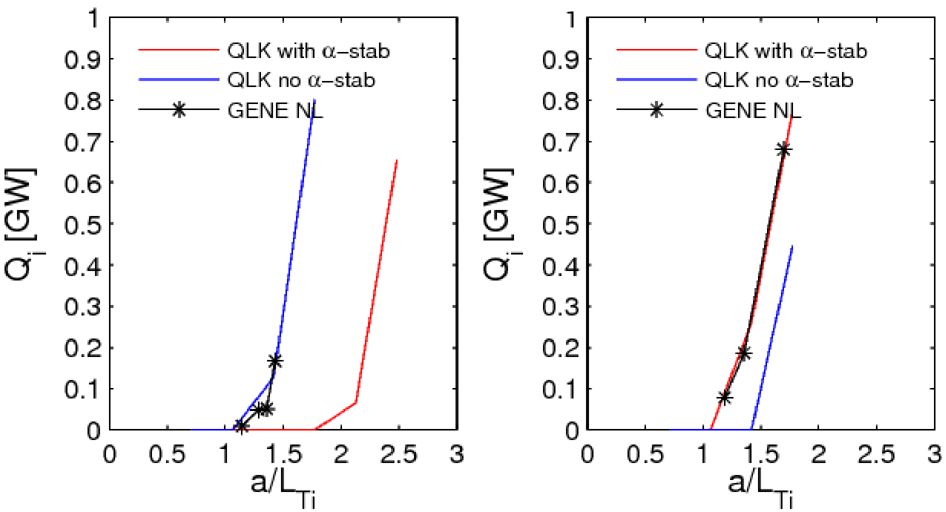


Specific challenges for QuaLiKiz in hybrid scenarios

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)

$\rho = 0.35,\ s = 0.24$ $\rho = 0.53,\ s = 0.94$



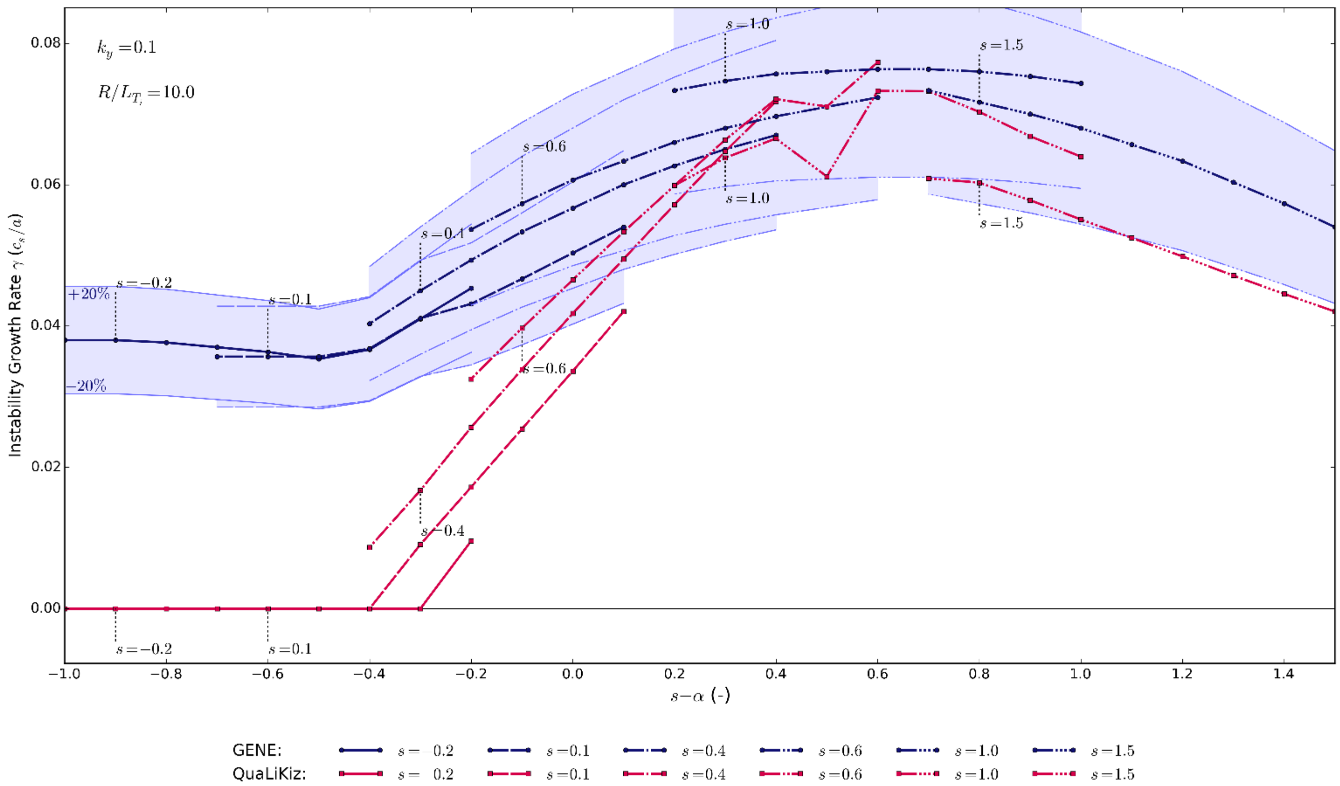
Threshold and stiffness agreement excellent for moderate magnetic shear (where it is actually destabilization).

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 $\rho > 0.5$
- Symmetry breaking from eigenfunction still maintained for momentum transport
- Baselines should be easier to model with QuaLiKiz (lower alpha, more electrostatic, sawteeth in inner core)

QuaLiKiz α-stabilization model not consistent at low $s-\alpha$

QLK vs linear-GENE comparison of α-stabilization

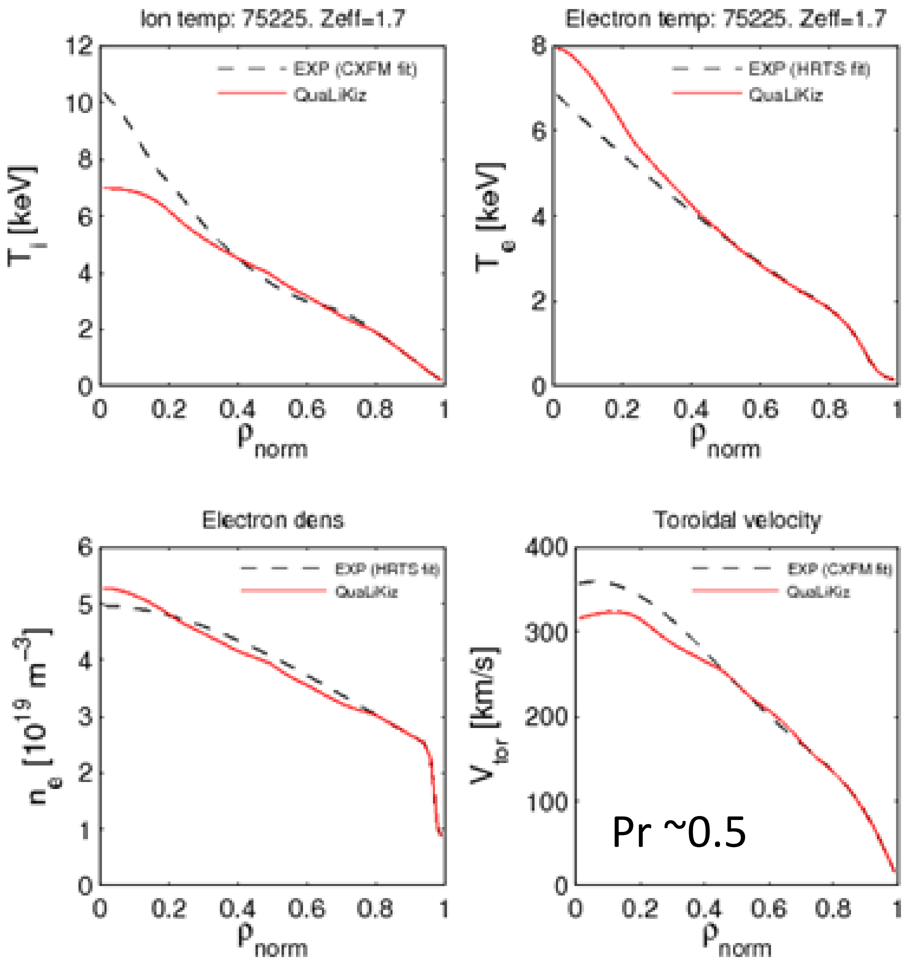


Caveats:
α-stabilization not kept for $\rho < 0.5$. QLK overpredicts stabilization compared to linear-GENE (plot by Oliver Linder). Likely due to extended eigenfunction in ballooning space in linear-GENE. Not captured by current QLK eigenfunction ansatz

In integrated modelling, $s-\alpha$ is clamped to a minimum = 0. Actually consistent with flat behaviour of GENE growth rates for low $s-\alpha$. More consistent solution under investigation

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

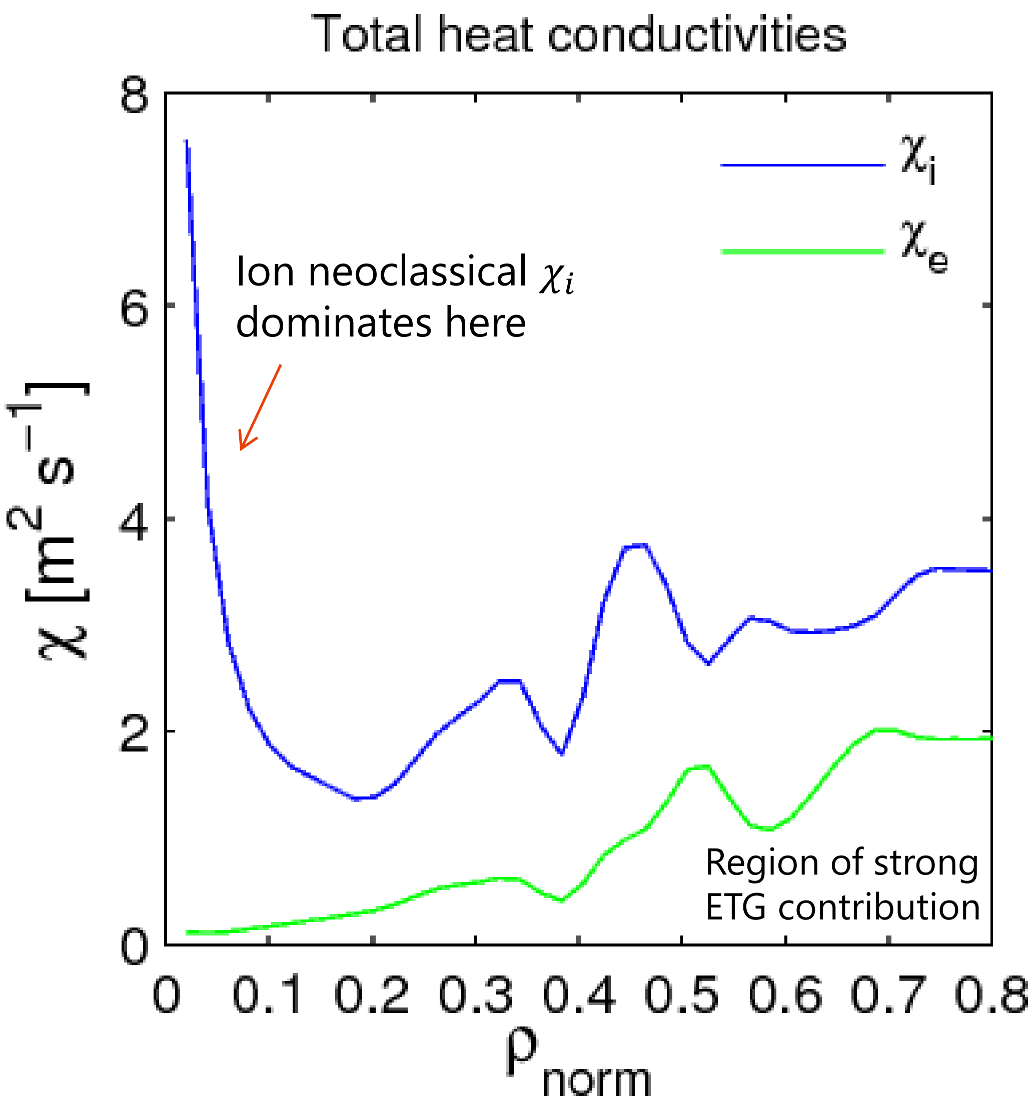
Boundary condition at $\rho = 0.8$

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

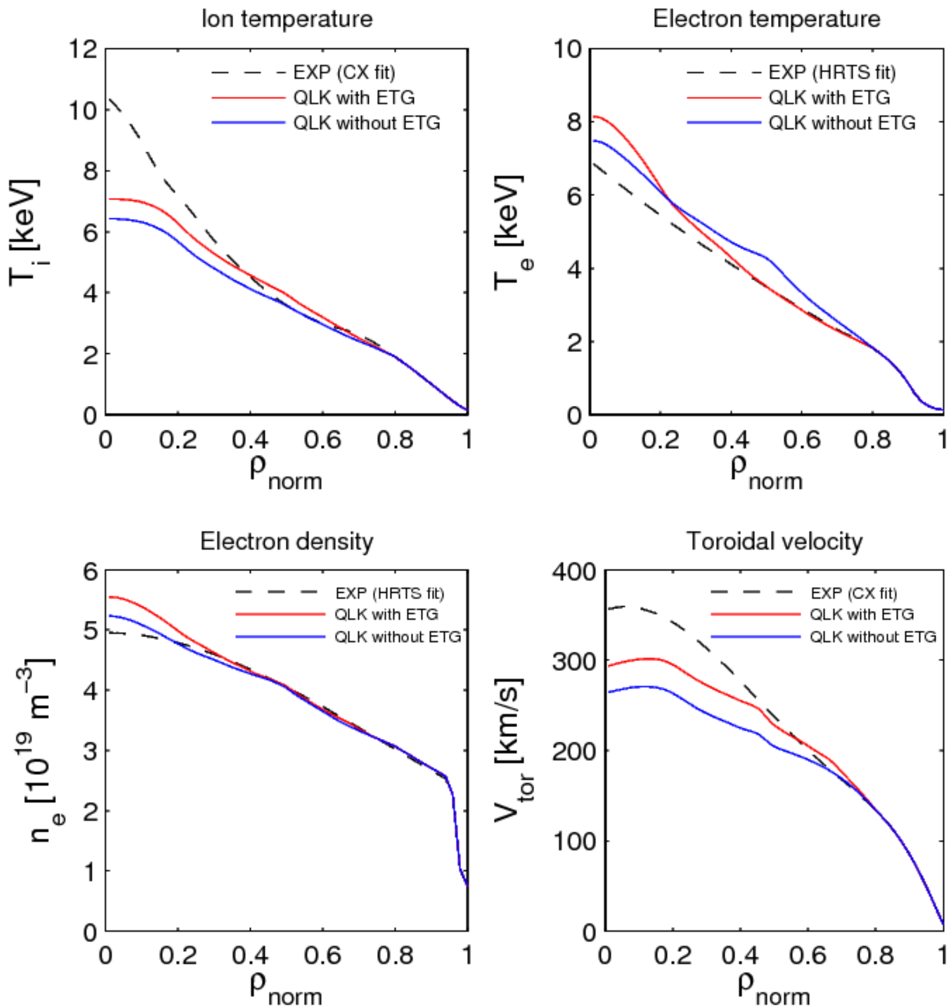
Heat conductivity prediction in flux matched NCLASS+ QLK, for hybrid scenario 75225



- Inner core ion heat dominated by neoclassical tranport
- ETG adjusted to N. Bonanomi JET work proved critical in edge. >Half of flux, avoids electron heat shortfall (as in e.g.Kinsey PoP 2015)
- Inner QLK boundary condition at $\rho = 0.15$, with linear extrapolation to $\rho = 0$

Sensitivity to ETG model in JET hybrid scenario integrated modelling

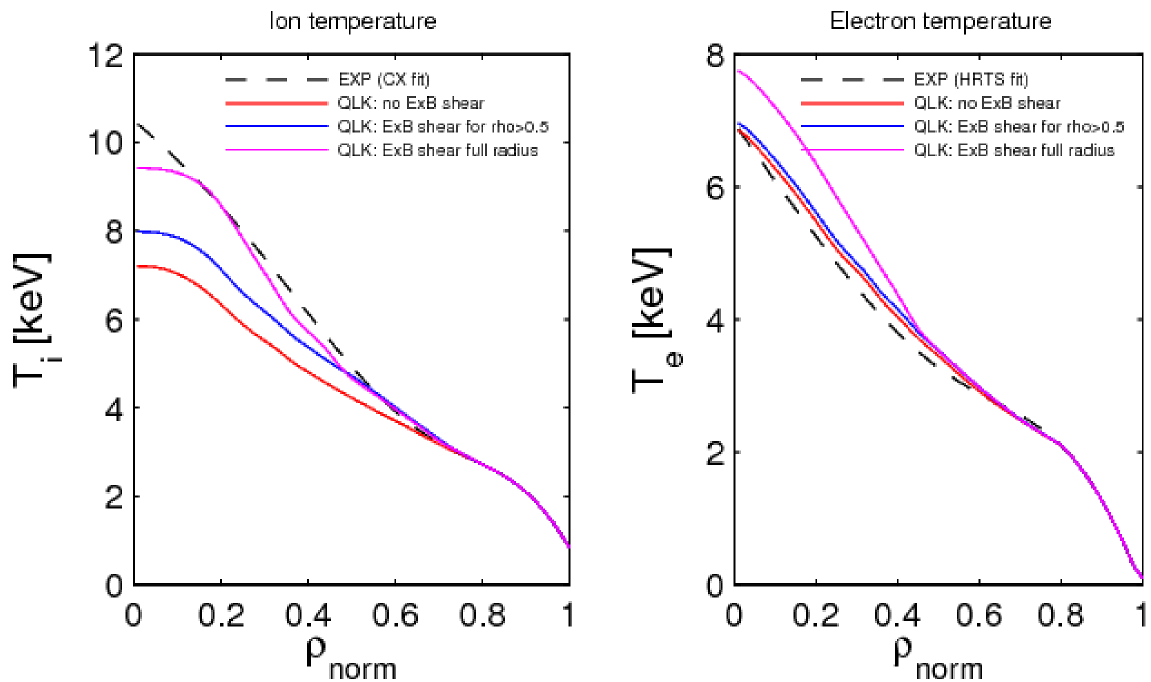
Comparison with and without ETG model



- ETG scales important for agreement (or, just a coincidence)

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

Sensitivity to rotation settings

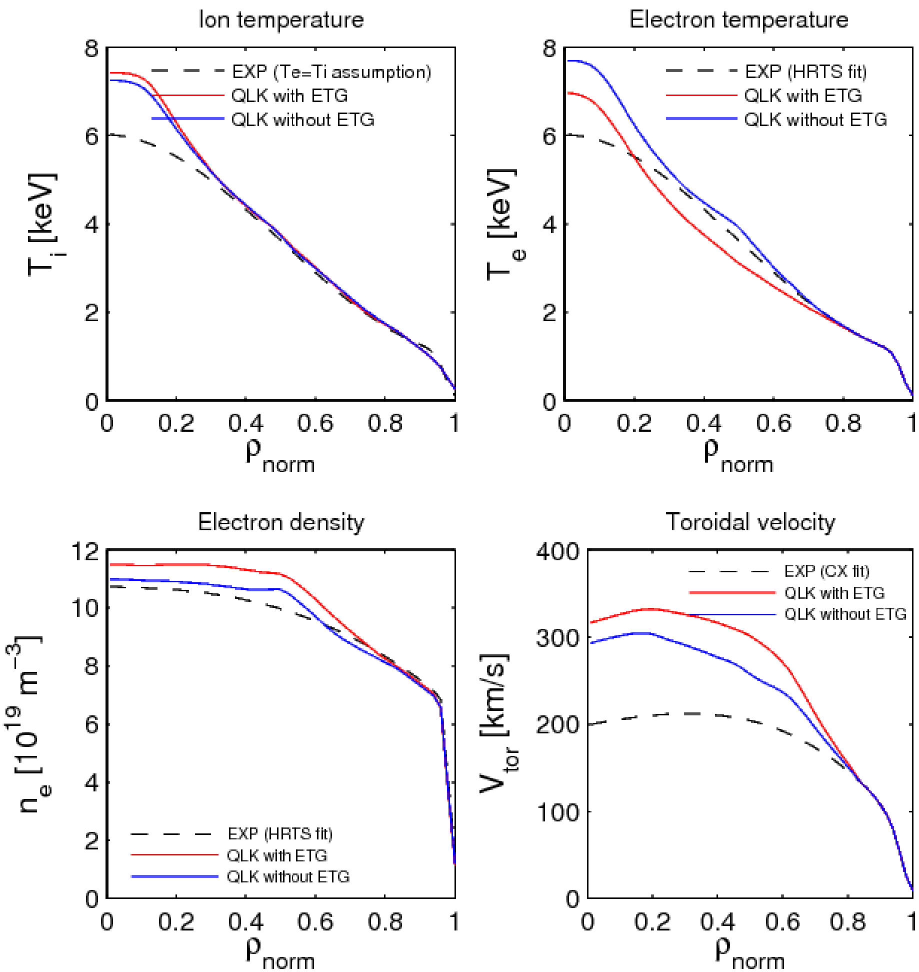


- ExB shearing not kept for $\rho < 0.5$ in integrated modelling
- "Agreement" with full rotation model is erroneous. NL simulations show that EM-stabilization is effective there, not ExB shear
- Due both to EM regime, and QLK likely underestimates parallel velocity gradient destabilization (under investigation)

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



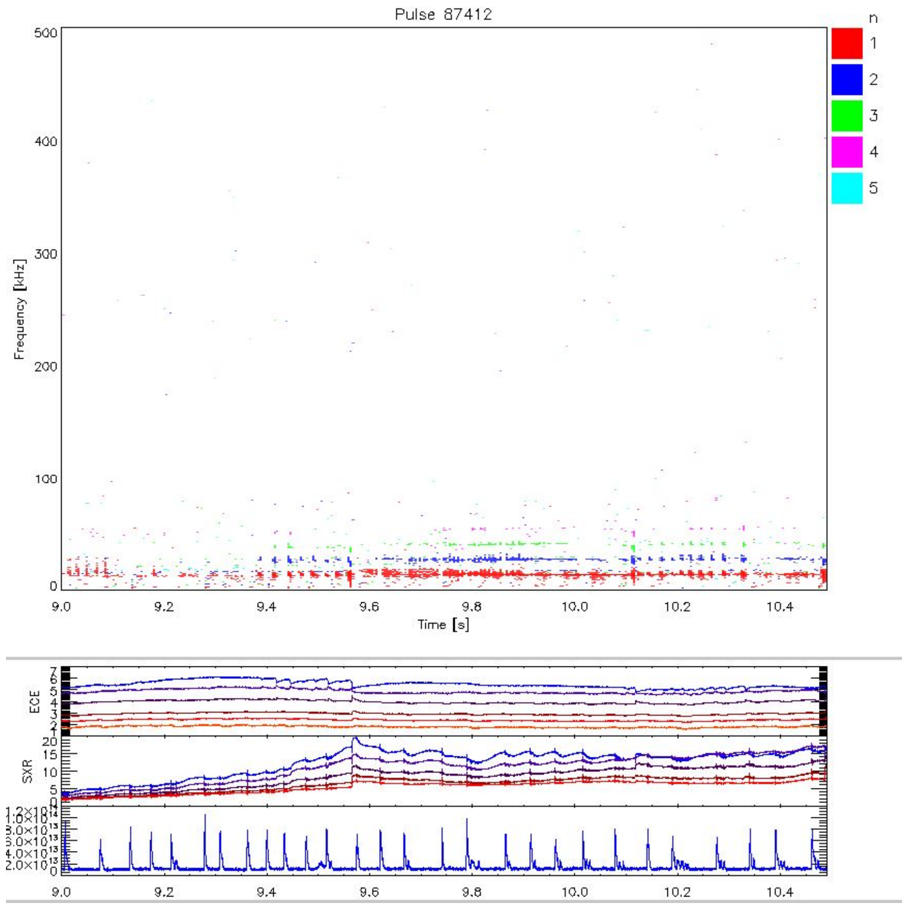
Good agreement in
All channels apart from V_{tor}

- Boundary condition at $\rho = 0.85$
- Stable for $\rho < 0.2$. No sawtooth model
- For comparson, T_i=T_e assumed due to poor inner core CX
- NTV torque due to NTMs flatten profile?
- ETG scales worsen agreement. ITG-ETG multiscale effects may be in different regime. Need multiscale model [1,2] in QuaLiKiz

[1] N.T. Howard *et al., 2016,* Phys. Plasmas 23, 056109
[2] G. Staebler *et al., 2016, accepted by PoP*

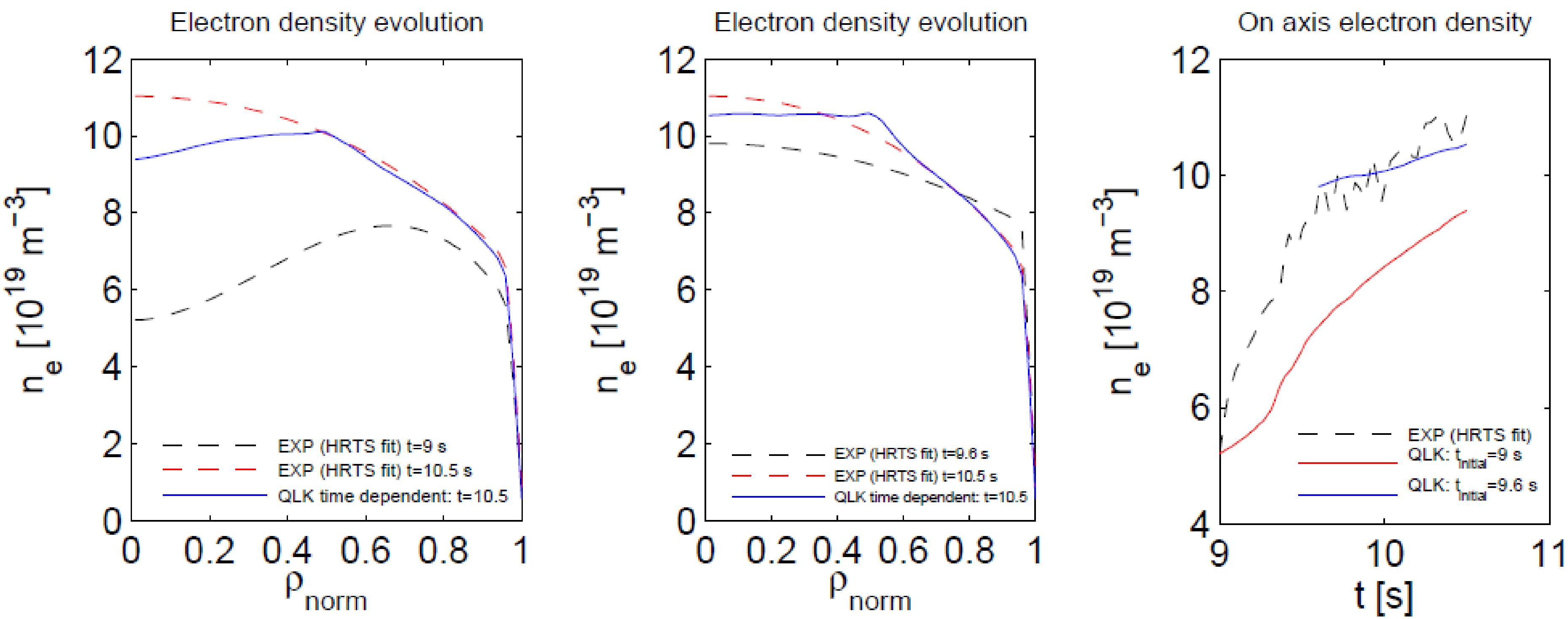
Are we missing an effective torque in our modelling, due to the presence of NTMs?

NTV torque due to NTMs flatten profile?
Modes present here in our time window 10-10.5s.
No modes in hybrid case where momentum transport well captured



Buildup of density following LH transition (mostly) recovered by QuaLiKiz

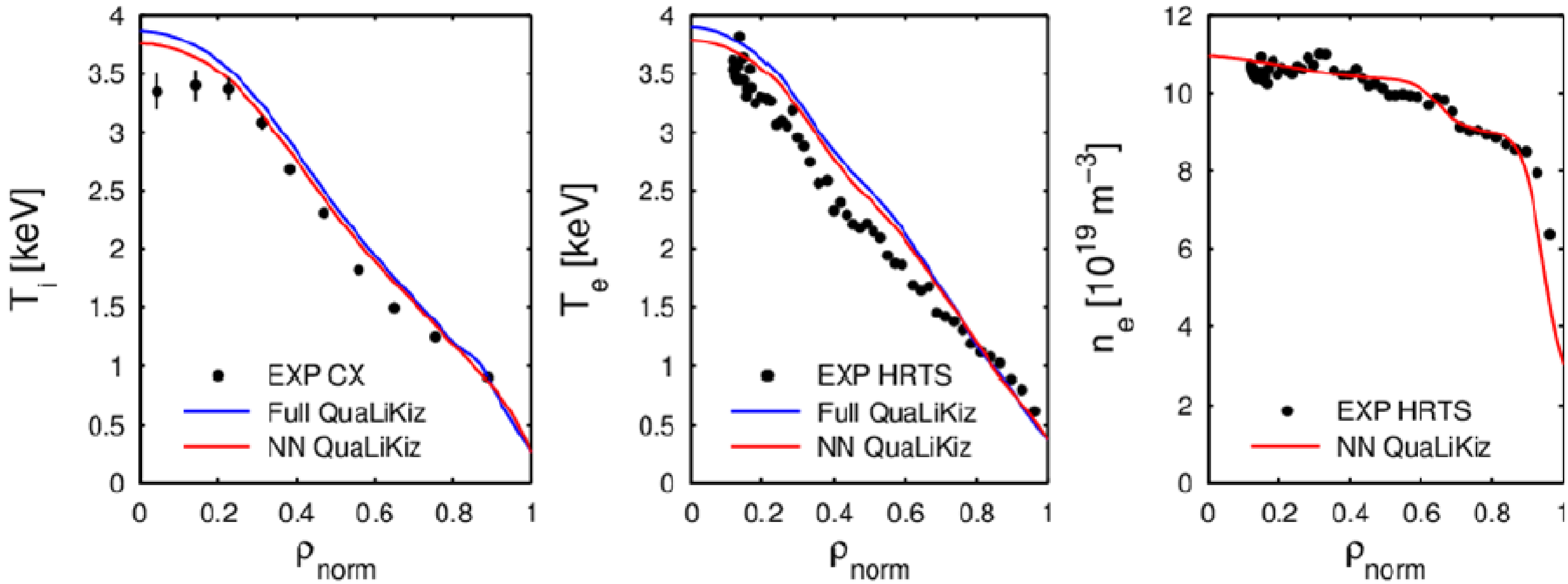
Dynamic simulation of density buildup following LH transition



Anomaly in early phase 9-9.6s. General trend well captured

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. Neural network fit and reproduces results $\times 10^6$ faster
- Already works surprisingly well on JET ITG dominated case in flux driven modelling
- In progress: Dense 11D input space population within ranges set by experiments.

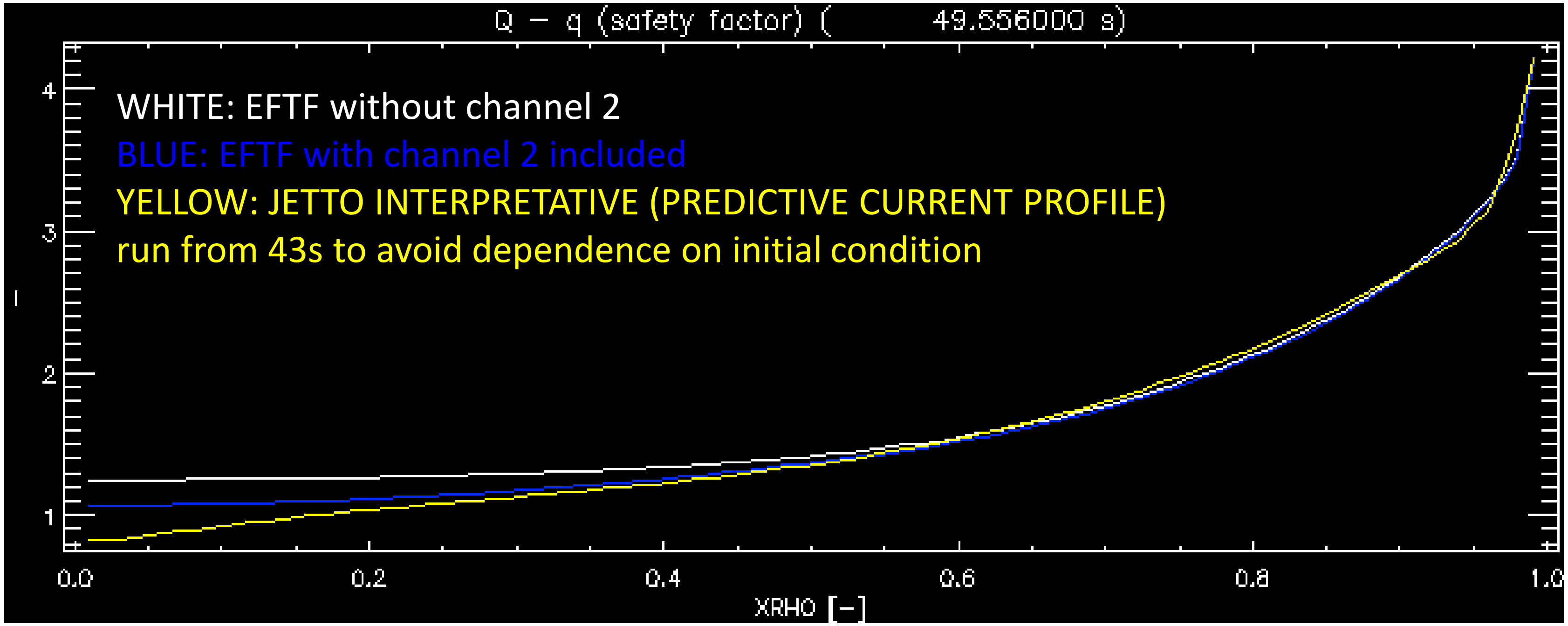
Summary

- First-principle-based transport model QuaLiKiz encouraging validation in JETTO-SANCO
- Successful C-wall hybrid scenario modelling, and now (mostly) successful ILW baseline case
- Working on more examples (S.Breton, C.Bourdelle).
  Ready for production runs and optimization (e.g. W-transport control, together with neoclassics)
- Caveats with regard to ExB model and α-stabilization. Workaround of only employing ExB shear and finite α for $\rho > 0.5$ is physically motivated by comparisons with GENE
- Open question regarding momentum transport modelling in presence of NTMs (thus NTV torque)
- Ongoing neural network emulation of QuaLiKiz (and quasilinear-GENE) for realtime capability

q-profile validated by interpretative modelling

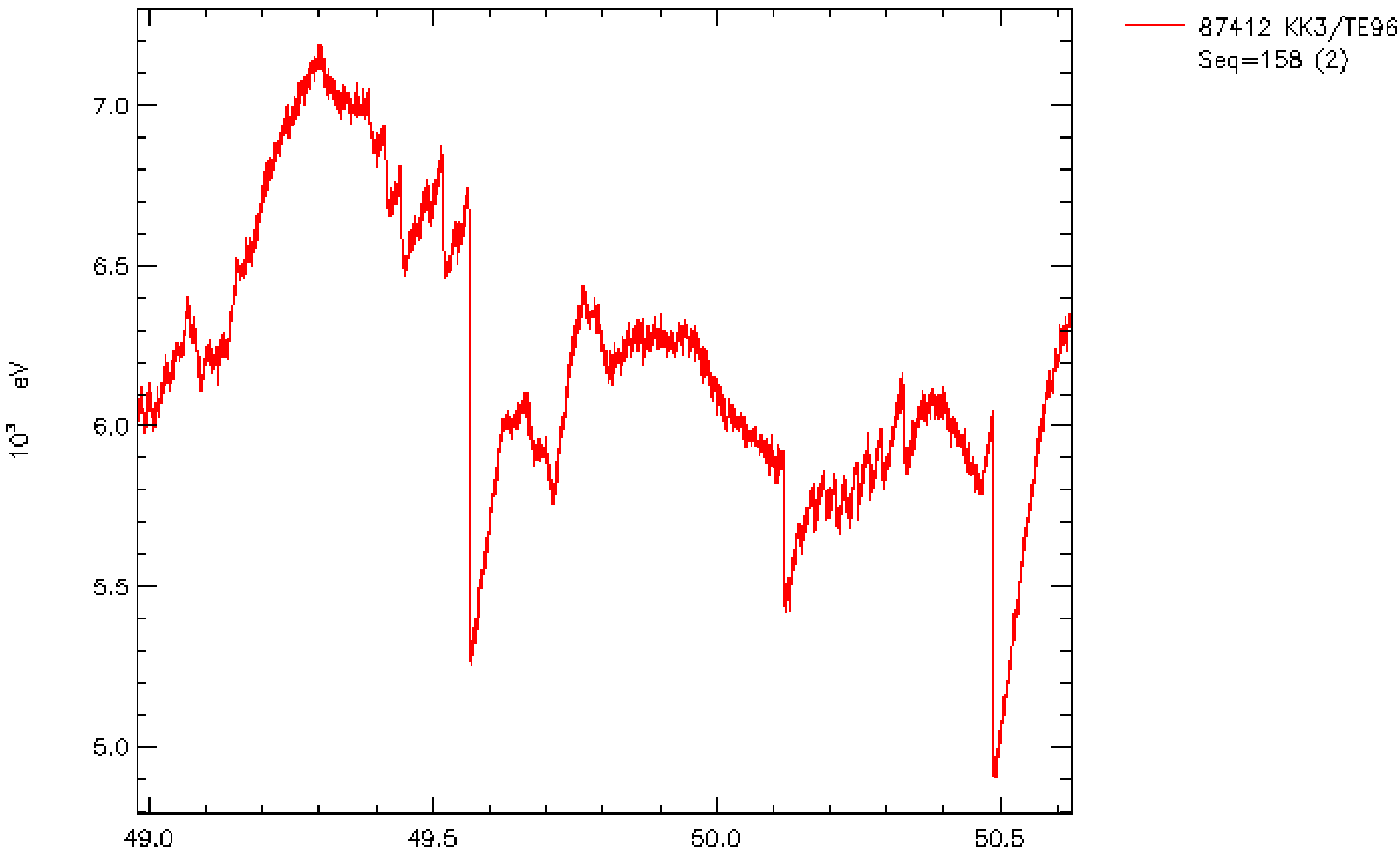
q-profile validation

From N. Hawkes – based on single timeslice comparison with MSE (only available at 48.5), it is likely that in the inner core, EFTF overpredicted q by around 0.2. Thus, our interpretative q-profile looks like it can be trusted.



Infrequent sawteeth in discharge

Largest sawtooth at 49.56s (from ECE data)



Sawteeth inversion radius an additional validation for q-profile modelling

Sawtooth inversion radius seen on KK3 channel 80

Corresponds to rhonorm~0.08, in agreement with interpretative q-profile