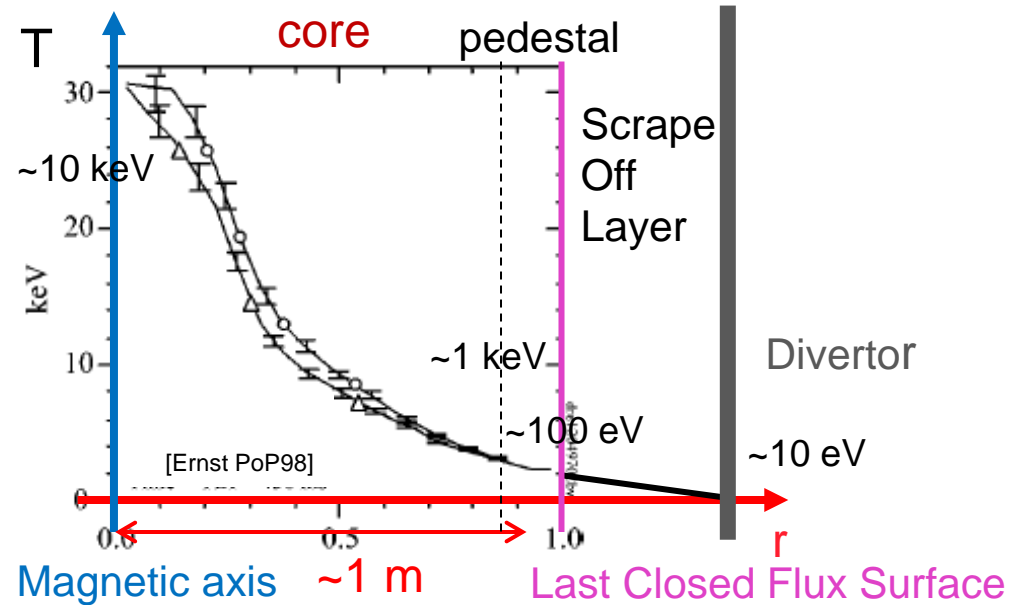
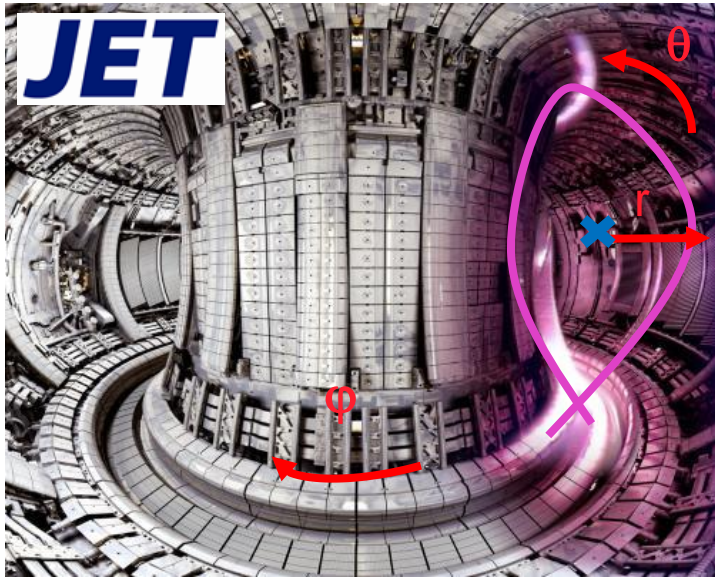


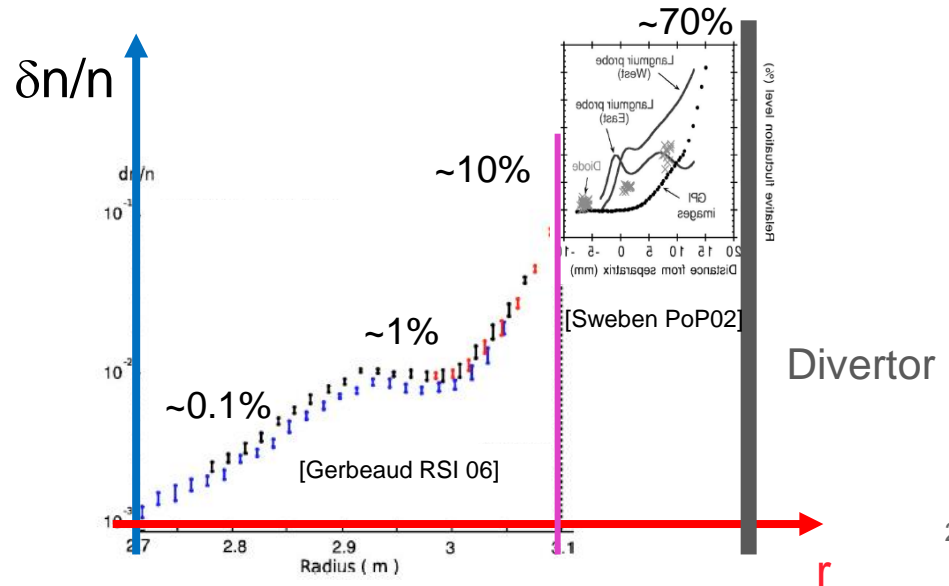
# **A TUTORIAL FOR QuaLiKiz USERS**

Clarisse Bourdelle, Jonathan Citrin

January 2018



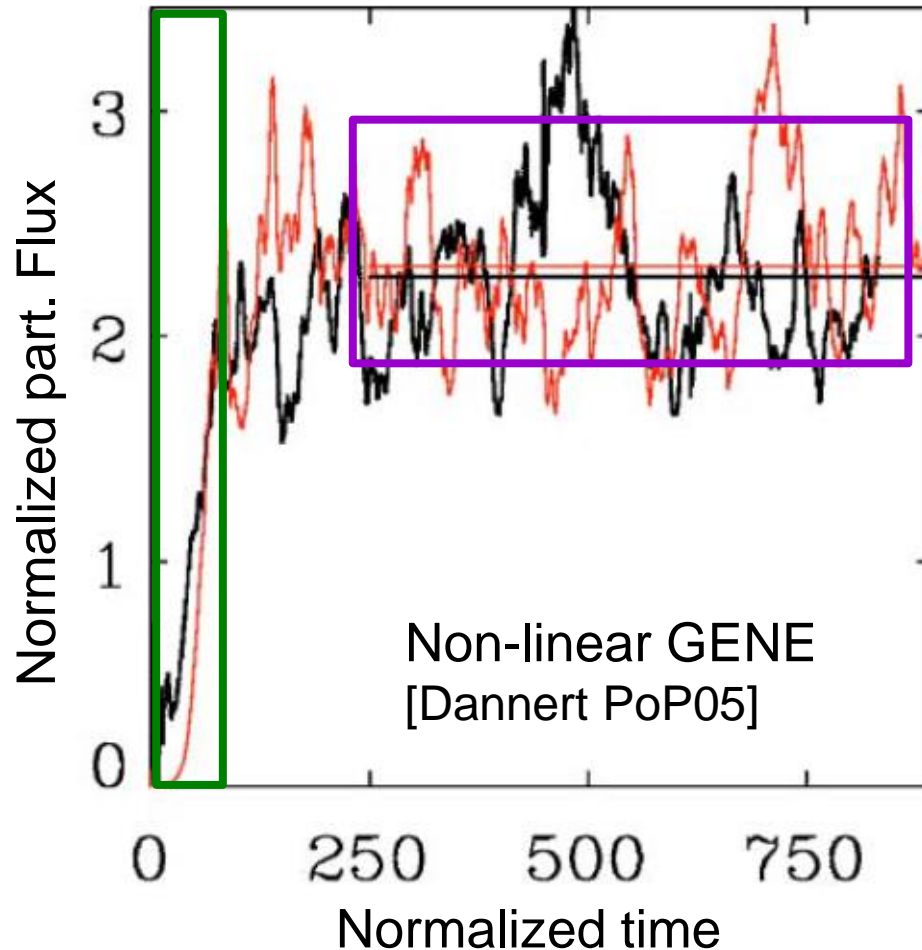
Large  $T$  and  $n$  gradients and curvature and  $B$  gradient  
→ turbulence  $\gg$  collisions  
governs transport  
To maximize  $\tau_E$  need to understand and predict turbulent transport



# INSTABILITY: LINEAR ONSET AND NON-LINEAR SATURATION

Linear phase

Saturated phase



Linear phase  
exponential growth as  $e^{\gamma t}$  gives info on  
instability threshold,  
parametric dependences

Saturated phase  
resulting from non-linear  
interactions between  
modes provides  
turbulent particle, heat,  
angular momentum  
fluxes

Ultimate goal: fast and first principle prediction of particle, heat, ang.  
momentum turbulent fluxes. Need to study linear phase first.

- Linear gyrokinetic formulation
- Linear stability and experimental observations
- Deriving and validating quasilinear particle, momentum and heat fluxes
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- Conclusions and perspectives

- In core of tokamak plasmas  $\frac{\delta n}{n} < \sim 1\%$  fluctuations  $\ll$  equilibrium distribution function of species s:  $f_s = f_{s,0} + \delta f_s$

electrostatic potential:  $\phi = \phi_0 + \delta\phi$  with:  $\delta\phi = \sum_{\vec{n}, \omega} \phi_{\vec{n}\omega}(\vec{J}) e^{i(\vec{n} \cdot \vec{\vartheta} - \omega t)}$ ,  
( $\vec{J}, \vec{\vartheta}$ ) the action and angle variables

$\omega = \omega_r + i\gamma$ ,  $\omega_r$  is the mode frequency and  $\gamma$  its growth rate

- $\delta\phi$  and  $\delta f_s$  related through 2 equations:

- Vlasov linearized,  $\delta f \times \delta\phi$  neglected

$$f_{\vec{n}\omega}(\vec{J}) = R_{lin}(\omega) \phi_{\vec{n}\omega}(\vec{J}) = -\vec{n} \cdot \frac{df_0(\vec{J})}{d\vec{J}} \frac{1}{\omega - \vec{n} \cdot \frac{d\vec{\vartheta}}{dt} + i0^+} e_s \phi_{\vec{n}\omega}(\vec{J})$$

- Maxwell for electrostatic case:  $\sum_s e_s n_s = 0$

→ **dispersion relation** in 6D :  $\sum_s e_s \langle R_{lin}(\omega) \phi_{\vec{n}\omega} \rangle = 0$

eigenfunction  $\phi_{\vec{n}\omega}$  and **eigenvalue**  $\omega = \omega_r + i\gamma$

- Due to large B, cyclotron frequency  $\omega >> \omega_c$  and Larmor radius  $\rho_L \ll L$

average on gyromotion:  $\phi_{\vec{n}\omega} \rightarrow \int \phi_{\vec{n}\omega} \frac{d\vartheta_L}{2\pi} \rightarrow 5D$

- 4D by assuming toroidal axisymmetry

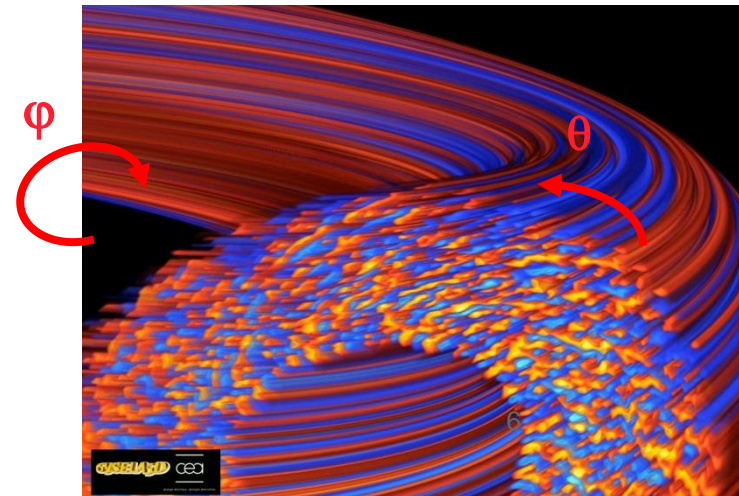
- Turbulent eddies elongated along B field lines:  $k_{\parallel} \ll k_{\perp}$

use field aligned coordinate  $\varphi - q(r)\theta$ ,

with  $q(r) \approx \frac{rB_{\varphi}}{RB_{\theta}}$

assume  $\phi_{\vec{n}\omega}$  ballooned around  $\theta = 0$

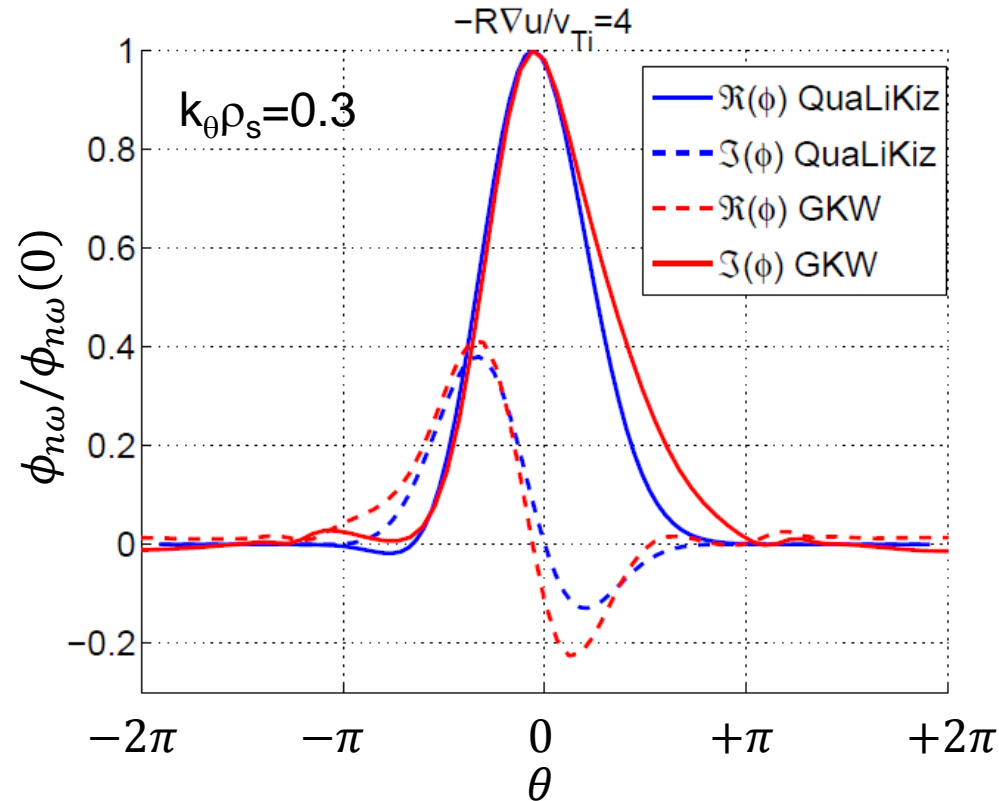
$\phi_{\vec{n}\omega}(r, \theta) \rightarrow \phi_{n\omega}(\theta) \equiv 3D$



GYSELA 5D [Grandgirard JCP06]

[Bourdelle, Garbet et al NF02; Bourdelle, Garbet et al PoP07]

- **eigenfunction in fluid limit**  
 $\omega \gg n \frac{d\vartheta}{dt}$  : a shifted Gaussian in **good agreement with self-consistent eigenfunc** from 4D code GWK [Peeters CPC09]
- $1/R$  and  $\nabla B$  drift and transit frequencies simplified, assuming very trapped/passing part. and circular concentric s- $\alpha$  mag. equi.  $\rightarrow$  2D integrals
- Efficient search of all eigenvalues in complex plane based on residue theorem [Davies JCP86]



[Cottier, Bourdelle et al PPCF14]



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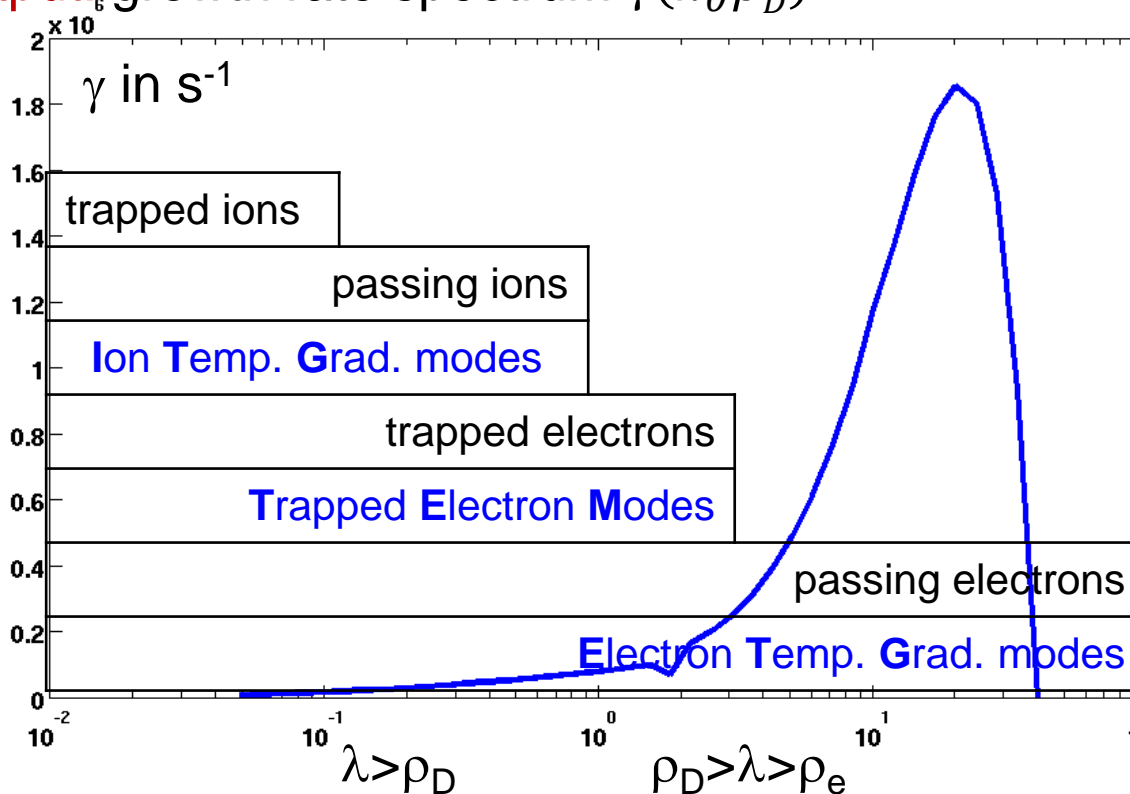


- To compute dispersion relation need:

$$\frac{r}{a}, \frac{R}{a}, \frac{\nabla n_s}{n_s}, \frac{\nabla T_s}{T_s}, \frac{\nabla U_{//}}{v_{th}/R}, \frac{U_{//}}{v_{th}}, \frac{\nabla E_r}{B} \frac{v_{th}}{R}, \frac{r \nabla q}{q}, q, \frac{T_i}{T_e}, \alpha, Z_{eff} \text{ from:}$$

- fitted experimental profiles, requires team work and care
- ad hoc values to explore parametric trends

- Output: growth rate spectrum  $\gamma(k_\theta \rho_D)$

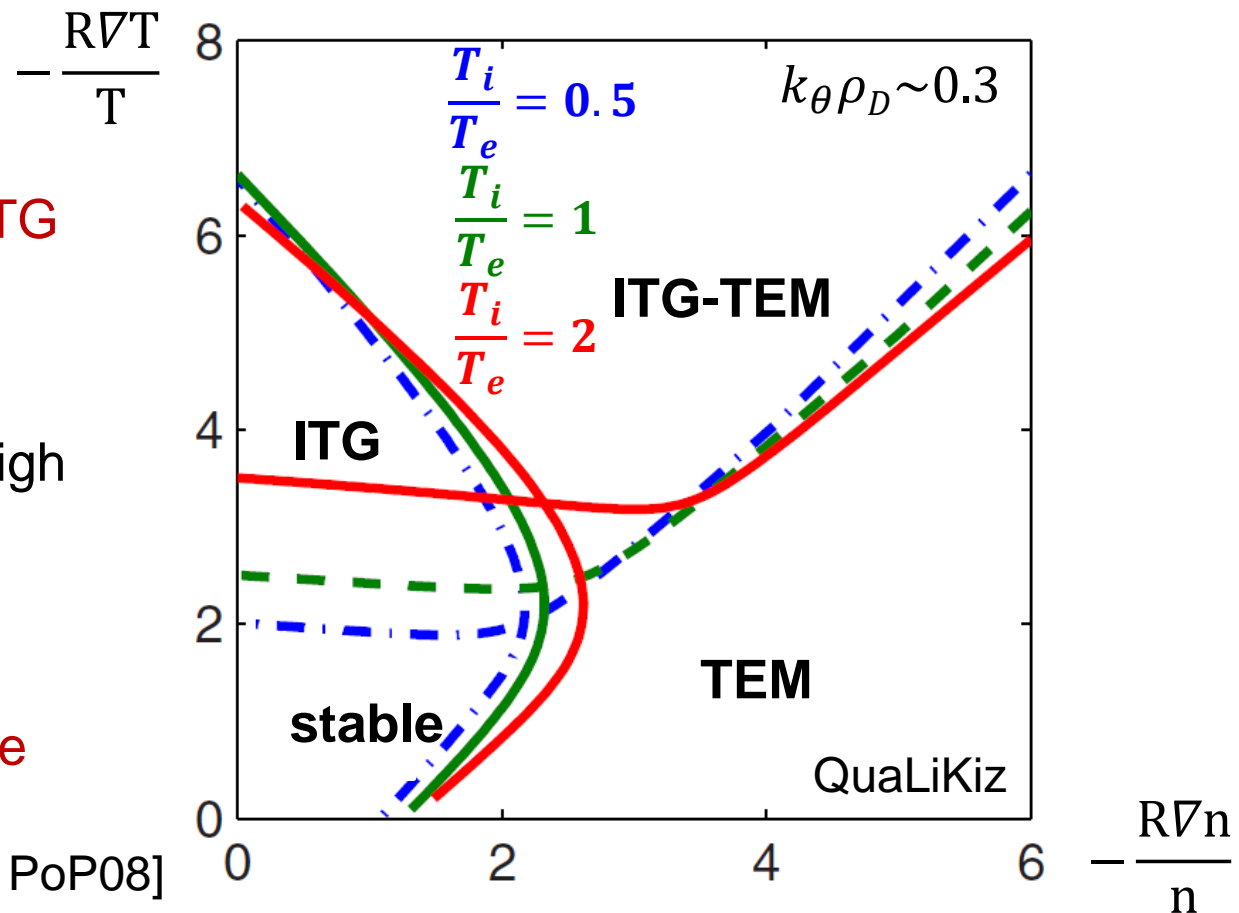


# ONSET OF UNSTABLE MODES ABOVE A T AND n THRESHOLD, ILLUSTRATION OF $T_i/T_e$ IMPACT

Large  $\frac{T_i}{T_e}$  stabilizing for ITG  
at low  $-\frac{R\nabla n}{n}$

but different impact at high  
 $-\frac{R\nabla n}{n}$  and on TEM  
threshold

→ need gyrokinetic code



[Casati, Bourdelle et al PoP08]

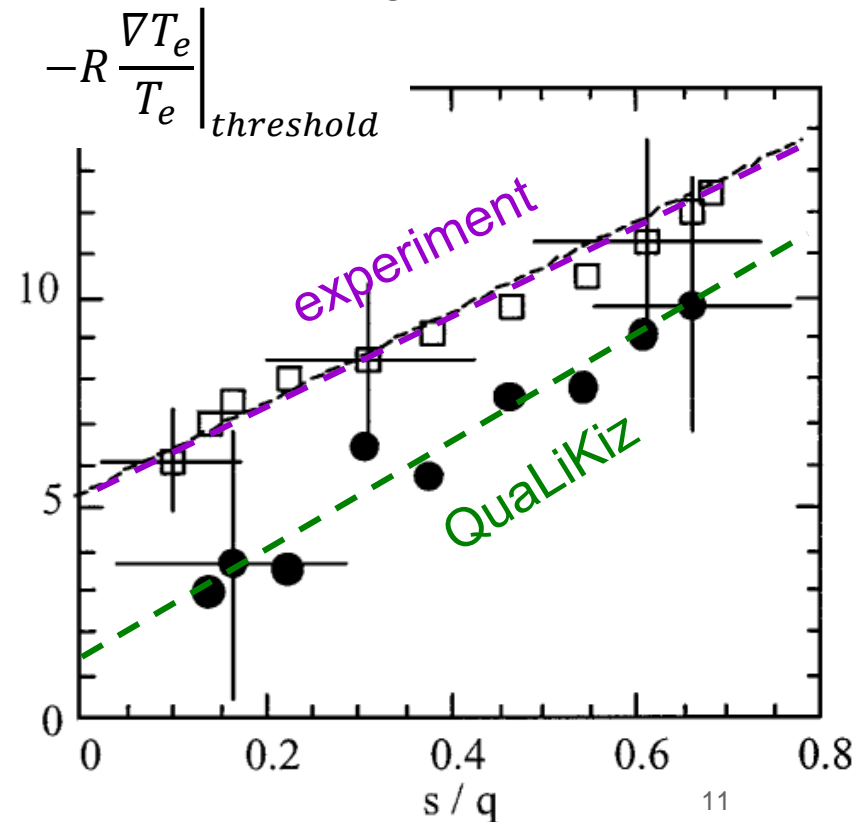
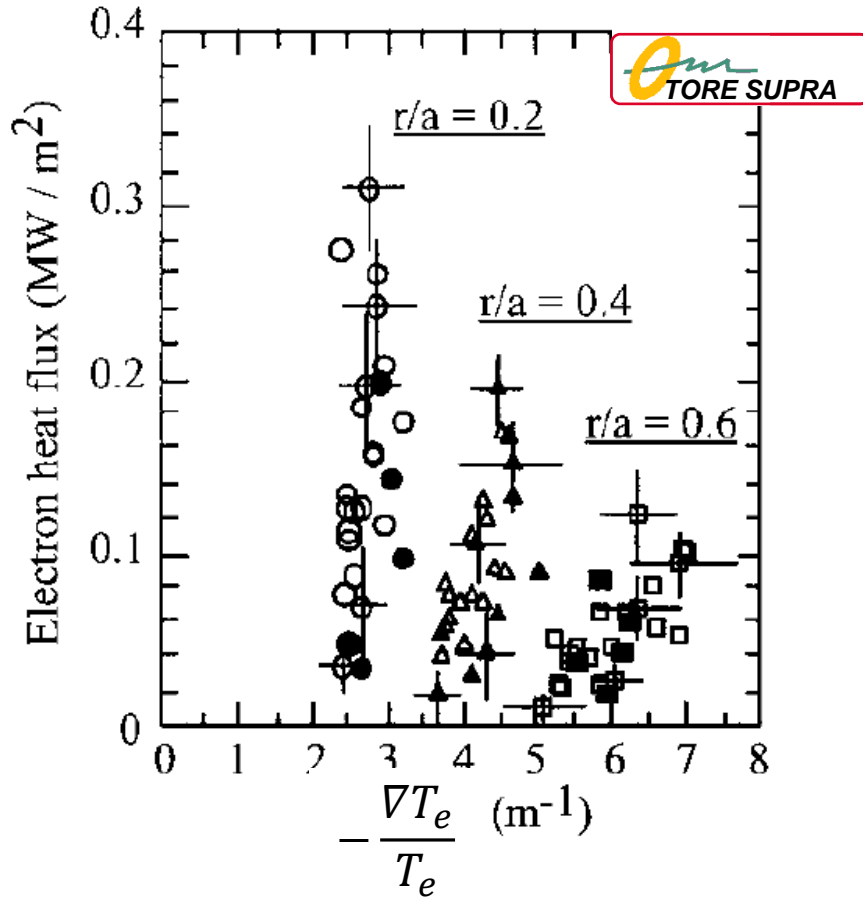
Threshold depends also on  $\frac{s}{q} = -\frac{r\nabla q}{q^2}$ ,  $Z_{eff}$ , etc

Stand alone analysis allow building up knowledge on turbulence trends

# EXPERIMENTAL PROOF OF EXISTENCE OF A CRITICAL TEMPERATURE THRESHOLD

- Expected electron T threshold observed experimentally in Tore Supra [Hoang PRL01], AUG [Ryter03], TCV [Camenen05], DIII-D [DeBoo05], etc
- $-R \left. \frac{\nabla T_e}{T_e} \right|_{threshold}$  increases with  $\frac{s}{q} = -\frac{r \nabla q}{q^2}$  as predicted

[Hoang, Bourdelle et al PRL01]



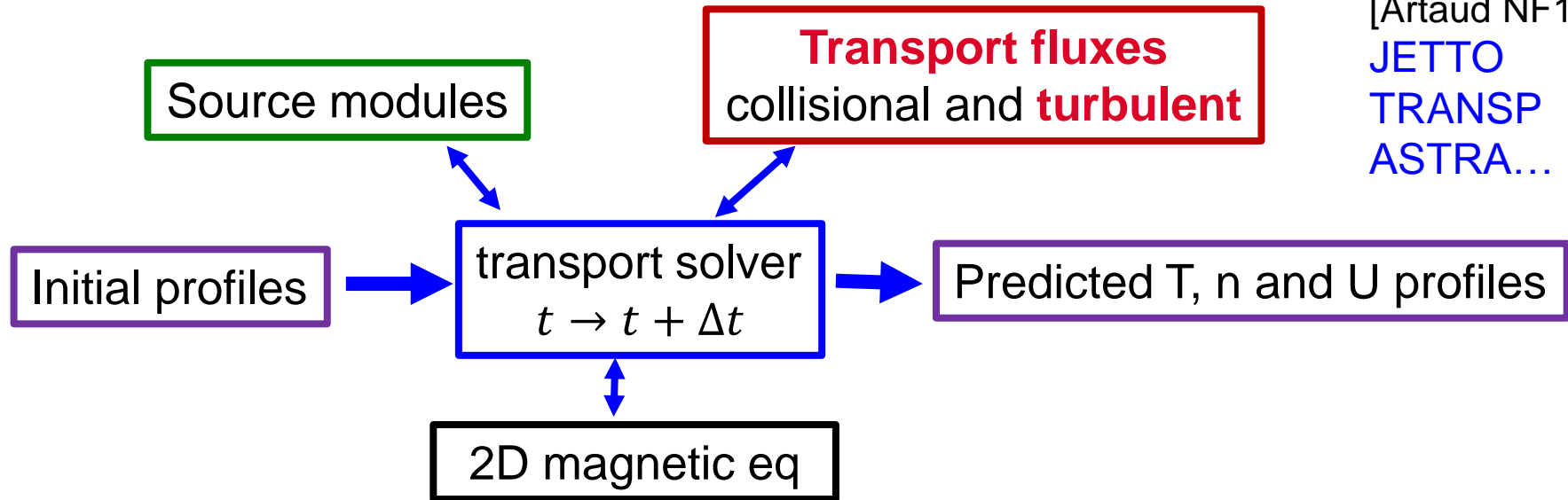
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# TOWARDS PREDICTING T, n AND U: CONSTRAIN ON COMPUTING TIME

$$\frac{\partial n}{\partial t} = -\vec{\nabla} \cdot \vec{\Gamma} + S = 0, \quad \Gamma = -D \nabla n + V n = \int_0^r S dr_1$$

For heat, particle or momentum:

**CRONOS**  
[Artaud NF10]  
**JETTO**  
**TRANSP**  
**ASTRA...**



$$t_{integrated\ sim.} = t_{turb.fluxes} \times \frac{1-1000\ s}{\Delta t_{transp.\ solver} \times 10^{-3}\ s} \times \frac{t_{discharge}}{1-10} \times N_{iterations}$$

$$t_{integrated\ sim.} \approx 10^4 \times t_{turb.fluxes}$$

# INTEGRATED MODELING NEEDS FAST AND FIRST PRINCIPLE TURBULENT FLUXES

Aim:  $t_{\text{integrated sim.}} \approx 10^4 \times t_{\text{turb.fluxes}} < \sim 24 \text{ h}$  on  $\sim 30$  CPU

need  $t_{\text{turb.fluxes}} < \sim 5 \text{ min}$  for 20 radial points and  $10 k_{\theta} \rho_s$

Gyrokinetic full-f flux driven	Gyrokinetic $\delta f$ gradient driven		Gyro-Landau fluid gradient driven
<b>GT5D</b> [Idomura POP06], <b>GYSELA</b> [Grandgirard JCP06]	<b>GS2</b> [Kotschenreuther PoP95], <b>GENE</b> [Jenko CPC00], <b>GYRO</b> [Candy-Waltz JCP03], <b>GKW</b> [Peeters CPC09]	additional approximations: electrostatic, $s-\alpha$ , etc: <b>QuaLiKiz</b> [Bourdelle, Garbet et al PoP07]	calibrated to gyro- kinetic theory <b>TGLF</b> [Staebler, Waltz et al PoP05, PoP10, PRL13]
<b>Nonlinear</b>		<b>Quasilinear</b>	
$\sim 10 \text{ Mh}$	$\sim 50\,000 \text{ h}$	$\sim 500 \text{ h}$	$\sim 30 \text{ s}$

easing interface with experiments

Other more approximated/faster fluid quasilinear models: Weiland/Multi-Mode Model [Weiland NF89, Rafiq PoP13] IFS-PPL [Kotschenreuther PoP95] GLF23 [Waltz PoP97]

$$\Gamma_s = \langle \delta f_s \delta V_E \rangle_\tau = \sum_{k_\theta, \omega, \omega_k} \text{Re} \left( \left\langle \delta f_s \frac{ik_\theta \delta \phi^*}{B} \right\rangle_\tau \right) \quad f_{n\omega} = R_{lin}(\omega) \phi_{n\omega}$$

$$\Gamma_s = - \sum_{k_\theta, \omega, \omega_k} \frac{k_\theta}{B} \text{Im} \langle R_{lin}(k_\theta, \omega, \omega_k) \rangle |\delta \phi(k_\theta, \omega, \omega_k)|^2$$

**quasi-linear flux** = **linear response** x **saturated potential**

Questions:

- Is the linear response valid?
- How to build the saturated potential?
- Test quasi-linear fluxes against non-linear sim. and experiments

Tools:

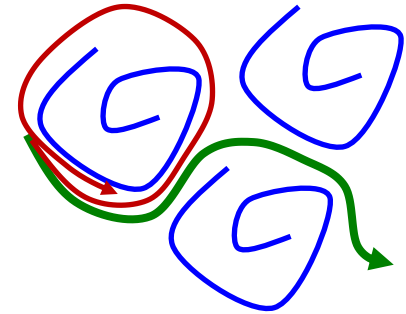
- Non-linear gyrokinetic simulations
- Turbulence measurements and experimental results



quasi-linear flux = linear response x saturated potential

Is it correct to neglect non-linear coupling  $\delta f \times \delta \phi$ ?

Turbulence auto-correlation time:  $\tau_{ac}$   
vs particle “flight” time:  $\tau_{flight} = \frac{\lambda_x}{\delta V_x} = \frac{\lambda_x}{\sqrt{\langle E_y^2 \rangle}/B}$



- If  $\tau_{ac} < \tau_{flight}$ ,  $K > 1$ , field trapping, need non-linear physics
- If  $\tau_{flight} < \tau_{ac}$ ,  $K < 1$ , linear response is sufficient

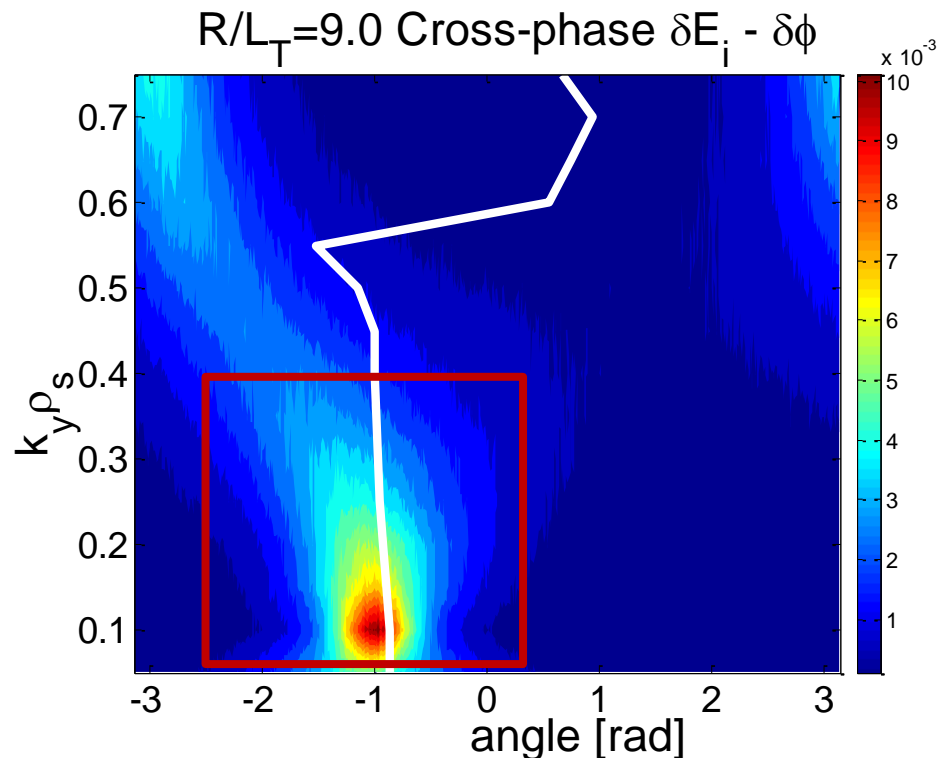
Run	$\sqrt{\langle E_y^2 \rangle}$	$\lambda_x$	$t_{ac}$	K
A: s=1	8.6	12.60	1.85	0.42
A: s=0.6	11.78	11.2	2.05	0.72
A: s=0.1	12.23	7.12	0.58	0.33
A: s=-0.4	9.66	6.94	1.85	0.86

**Non-linear GENE**

[Citrin, Bourdelle et al PoP12]

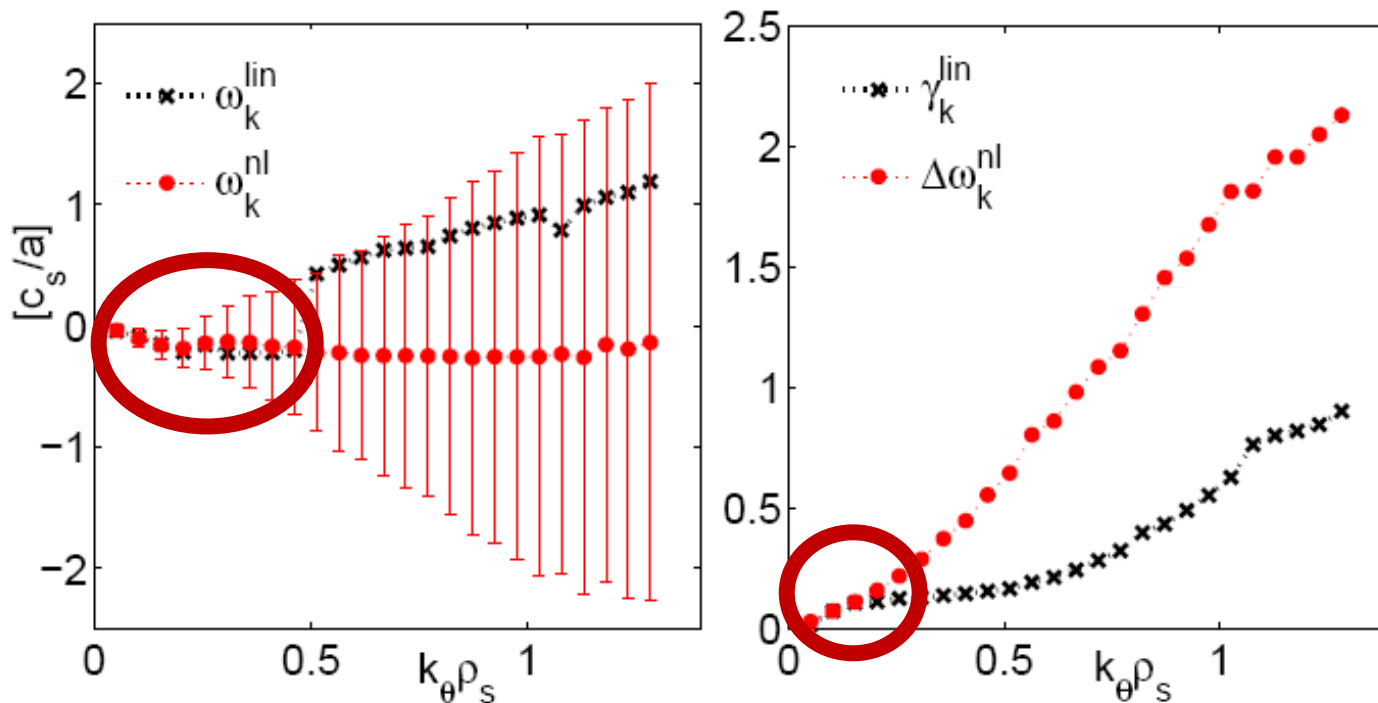
quasi-linear flux = linear response x saturated potential

cross phase of linear response vs  
PDF of non-linear cross phase:  $\Gamma_{NL}/\delta\phi^2$



**agreement** at low  $k_y \rho_s$   
where most of transport

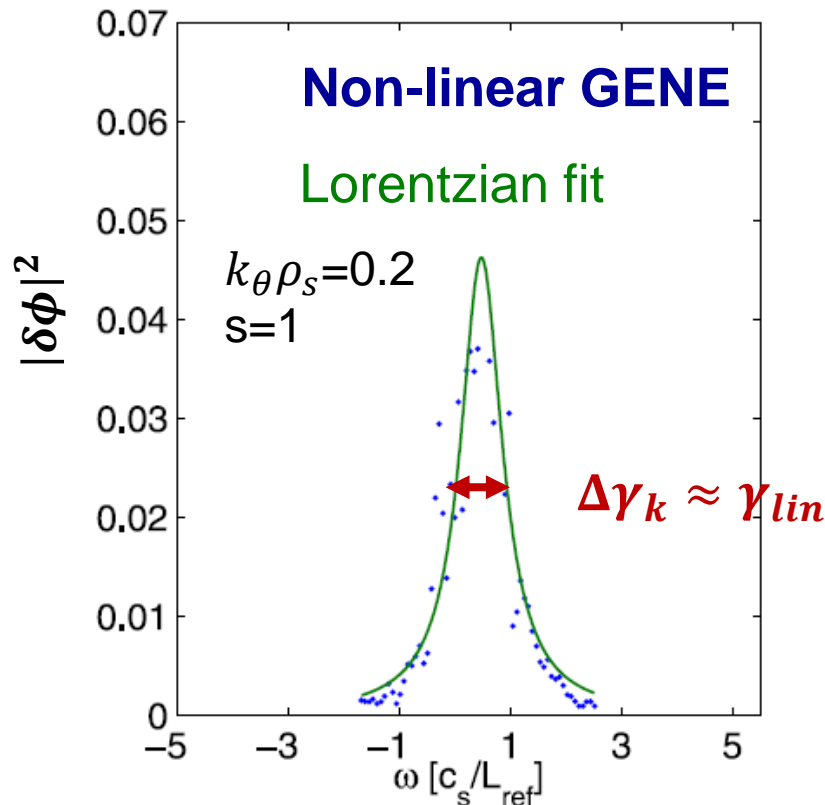
quasi-linear flux = linear response x saturated potential



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

quasi-linear flux = linear response x **saturated potential**

$$\text{Im}\langle R_{lin}(k_\theta, \omega, \omega_k) \rangle \propto \text{Im} \left( \frac{1}{\omega - n \frac{d\vartheta}{dt} + i\Delta\gamma_k} \right) = \frac{\Delta\gamma_k}{\left( \omega - n \frac{d\vartheta}{dt} \right)^2 + (\Delta\gamma_k)^2}$$



Frequency broadening: **Lorentzian** of **width  $\Delta\gamma_k \approx \gamma_{lin}$**  at low  $k_\theta \rho_s$  but at higher  $k_\theta \rho_s$  and for  $|s| < 0.6$  interplay with zonal flow and probably with damped mode modify  $\Delta\gamma_k$

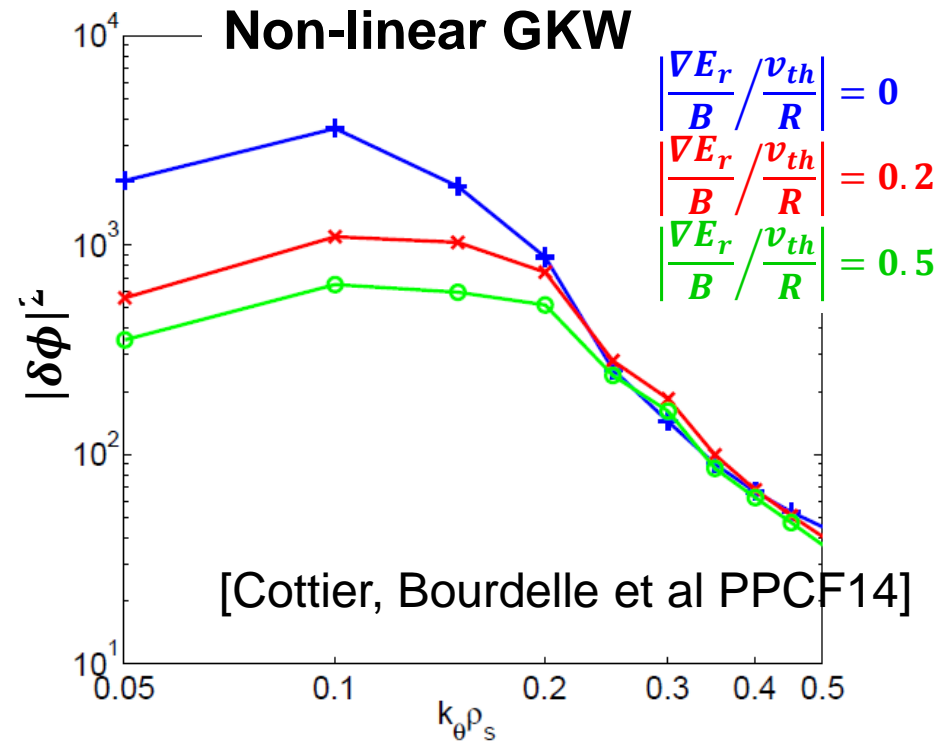
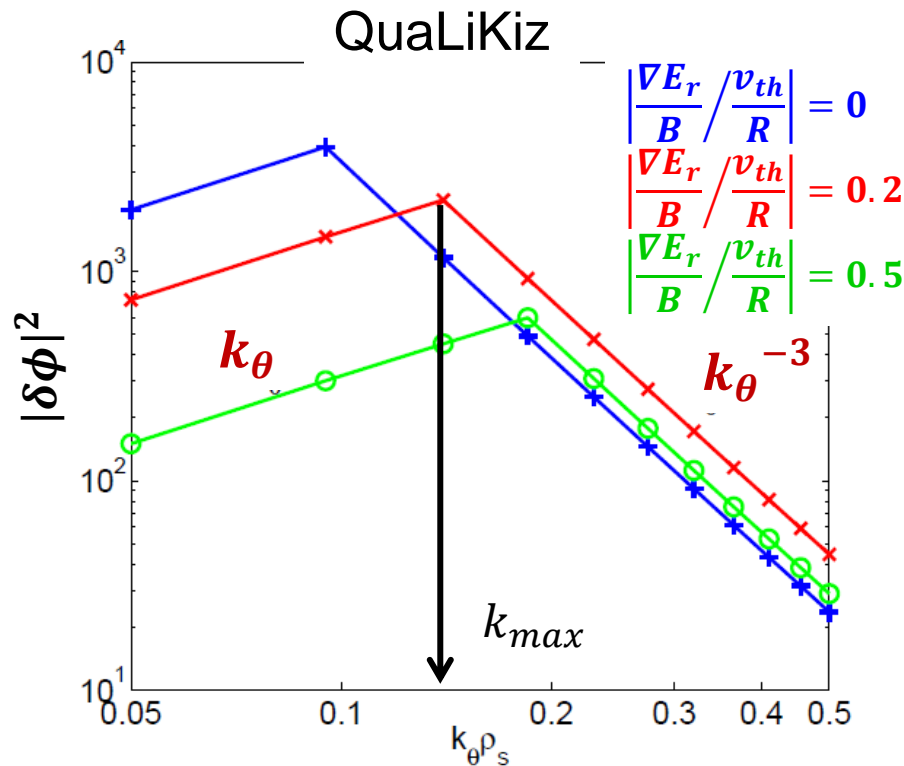
Lack of 1<sup>st</sup> principle theoretical model  
→ **ad-hoc renormalization factor** for  $|s| < 0.6$

[Citrin, Bourdelle et al PoP12]

**quasi-linear flux = linear response x saturated potential**

Mixing length rule:  $\max \left( D_{eff} \approx \frac{R\Gamma_s}{n_s} \right) \Big|_{k_{max}} = \frac{\gamma_{lin}}{\langle k_{\perp}^2 \rangle} \Big|_{k_{max}} \propto \max(|\delta\phi|^2)$

$\langle k_{\perp}^2 \rangle = k_{\theta}^2 (1 + (s - \alpha)^2 \langle \theta^2 \rangle)$  with  $\langle \theta^2 \rangle = \frac{\int \theta^2 \phi_{n\omega}(\theta) d\theta}{\int \phi_{n\omega}(\theta) d\theta}$  and  $\phi_{n\omega}(\theta)$  lin. eigenfunc.



Can reproduce ExB shear impact reducing  $\max(|\delta\phi|^2)$  and shifting it to larger  $k_{\theta} \rho_s$

**quasi-linear flux = linear response x saturated potential**

From  $\sum_{k_\theta, \omega, \omega_k} \text{Re} \left( \left\langle \delta f_s \frac{ik_\theta \delta \phi^*}{B} \right\rangle_\tau \right)$

get **particle flux**:

$$\Gamma_s = \sum_{k_\theta, \omega, \omega_k} \text{Re} \left( \left\langle \delta n_s \frac{ik_\theta \delta \phi^*}{B} \right\rangle_\tau \right)$$

**energy flux**:

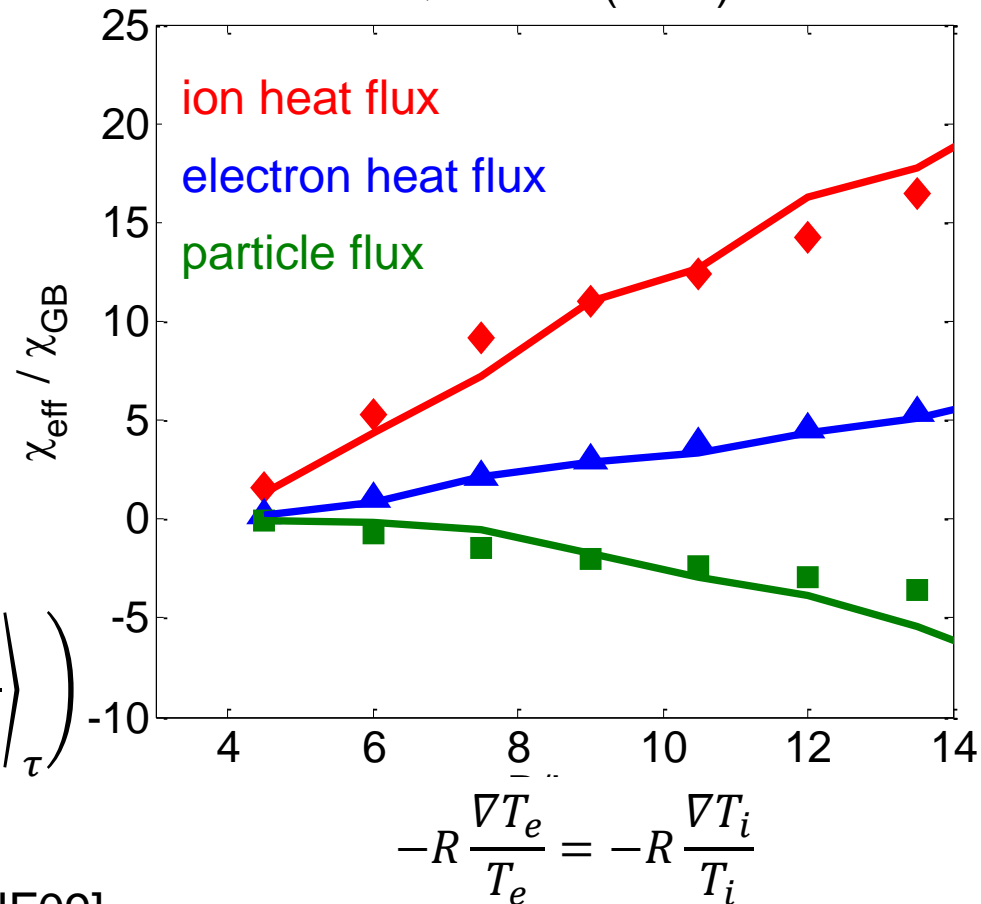
$$Q_s = \sum_{k_\theta, \omega, \omega_k} \text{Re} \left( \left\langle \frac{3}{2} \delta P_s \frac{ik_\theta \delta \phi^*}{B} \right\rangle_\tau \right)$$

**parallel ang. momentum flux**:

$$\Pi_{//} = \sum_{s, k_\theta, \omega, \omega_k} \text{Re} \left( \left\langle m_s R v_{//} \delta n_s \frac{ik_\theta \delta \phi^*}{B} \right\rangle_\tau \right)$$

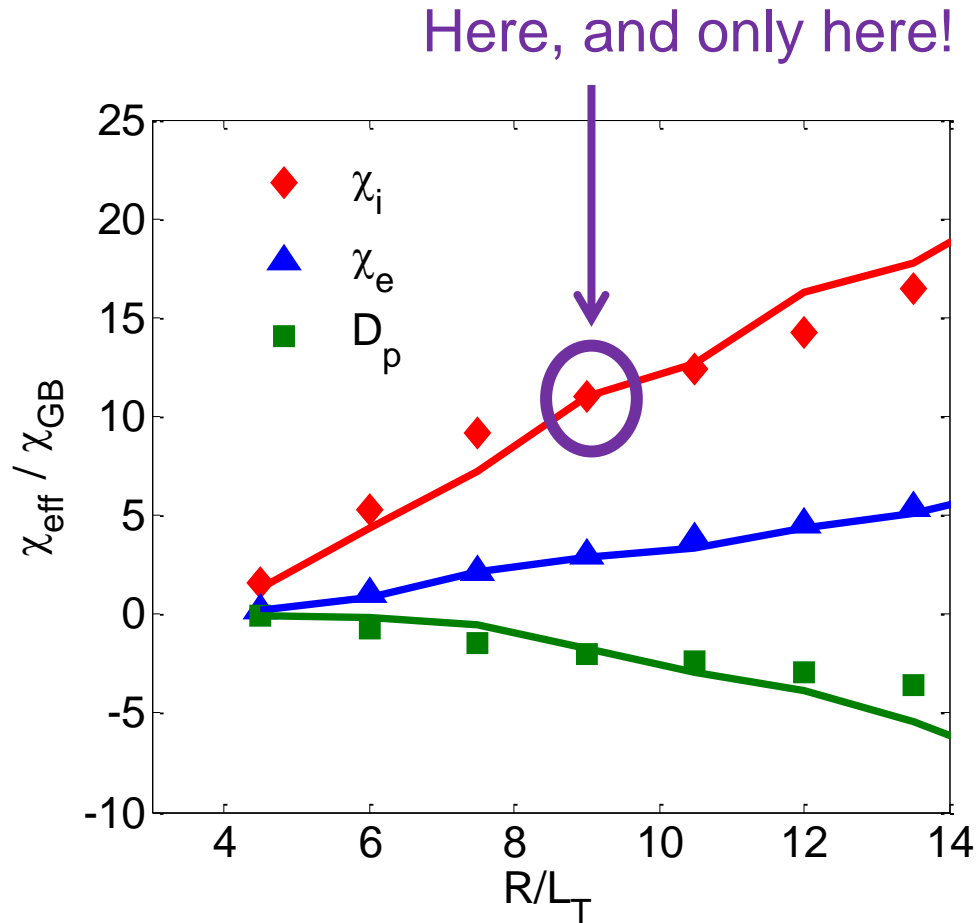
**Non-linear GYRO (symbols)**

**QuaLiKiz (lines)**



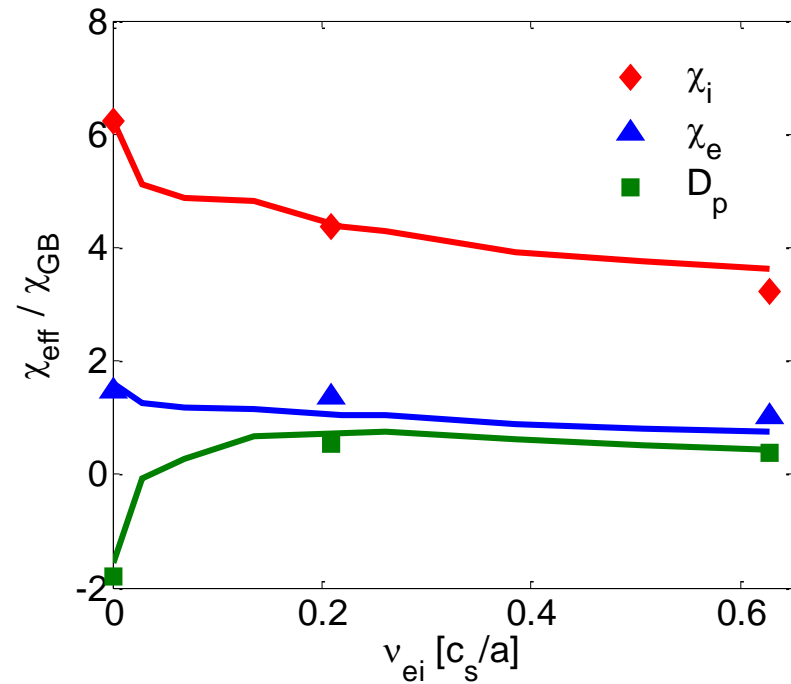
[Casati, Bourdelle et al NF09]

# WHERE IS THE TUNING DONE??



i.e. on GA standard case  
ion heat flux only!

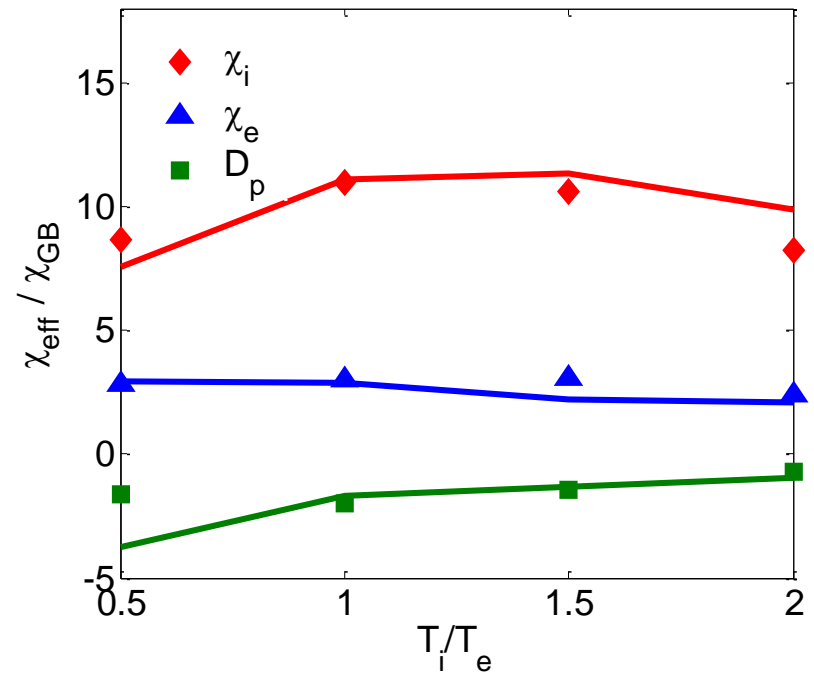




## Collisionality scan on Tore Supra parameters

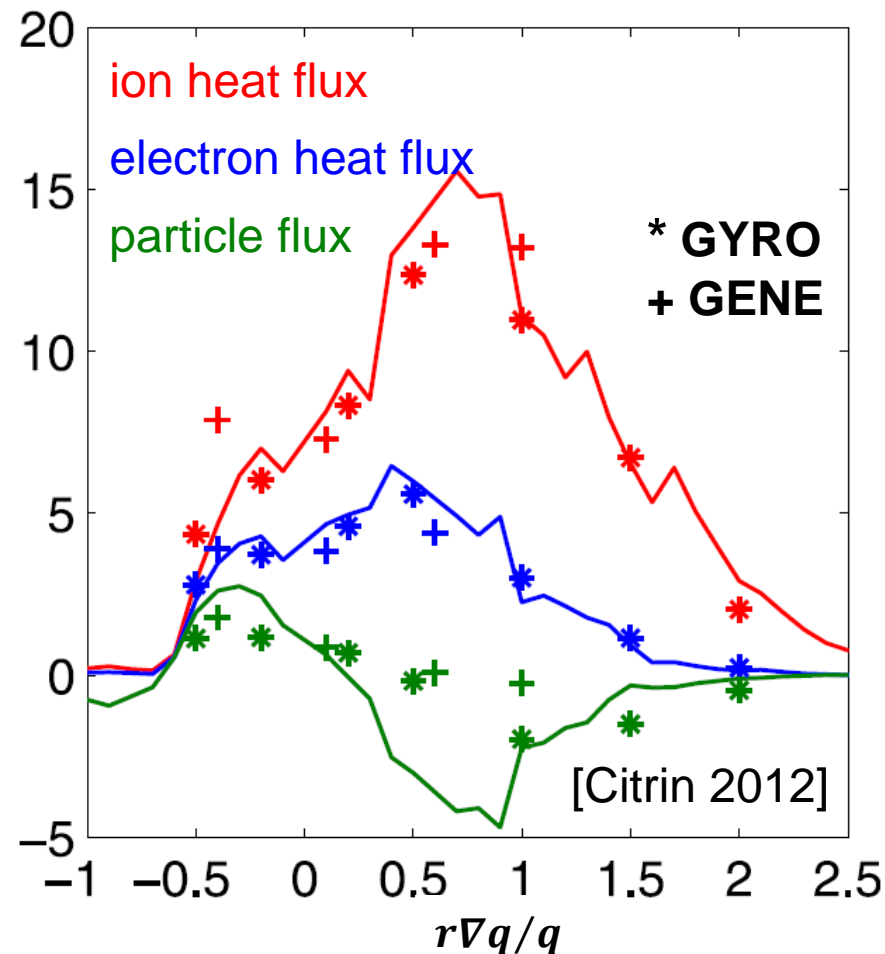
$v^*$  session:  $r/a=0.5$ ,  $\rho^*=1/500$ ,  
 $R/L_{Ti}=10.5$ ,  $R/L_{Te}=13.4$ ,  $R/L_n=4.5$ ,  
 $q=2.0$ ,  $s=1.3$ ,  $T_i/T_e=1.0$

A. Casati et al., Nucl. Fus. 2009

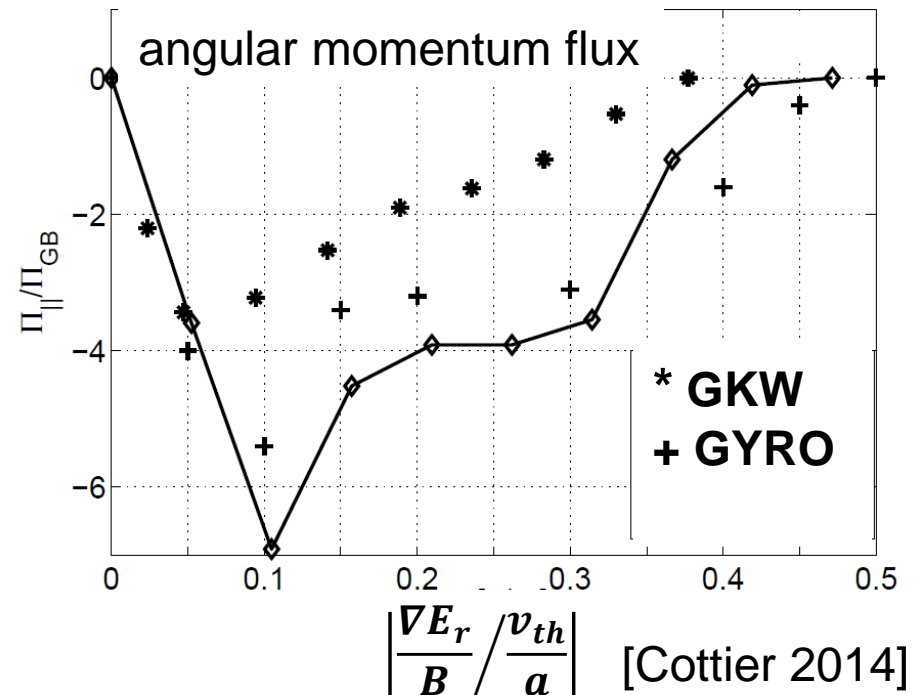


## $T_i/T_e$ scan on GA-std case

GA-std case:  $r/a=0.5$ ,  $\rho^*=1/400$ ,  
 $R/L_{Ti}=R/L_{Te}=9.0$ ,  $R/L_n=3.0$ ,  $q=2.0$ ,  
 $s=1.0$ ,  $v_{ei}=0.0$



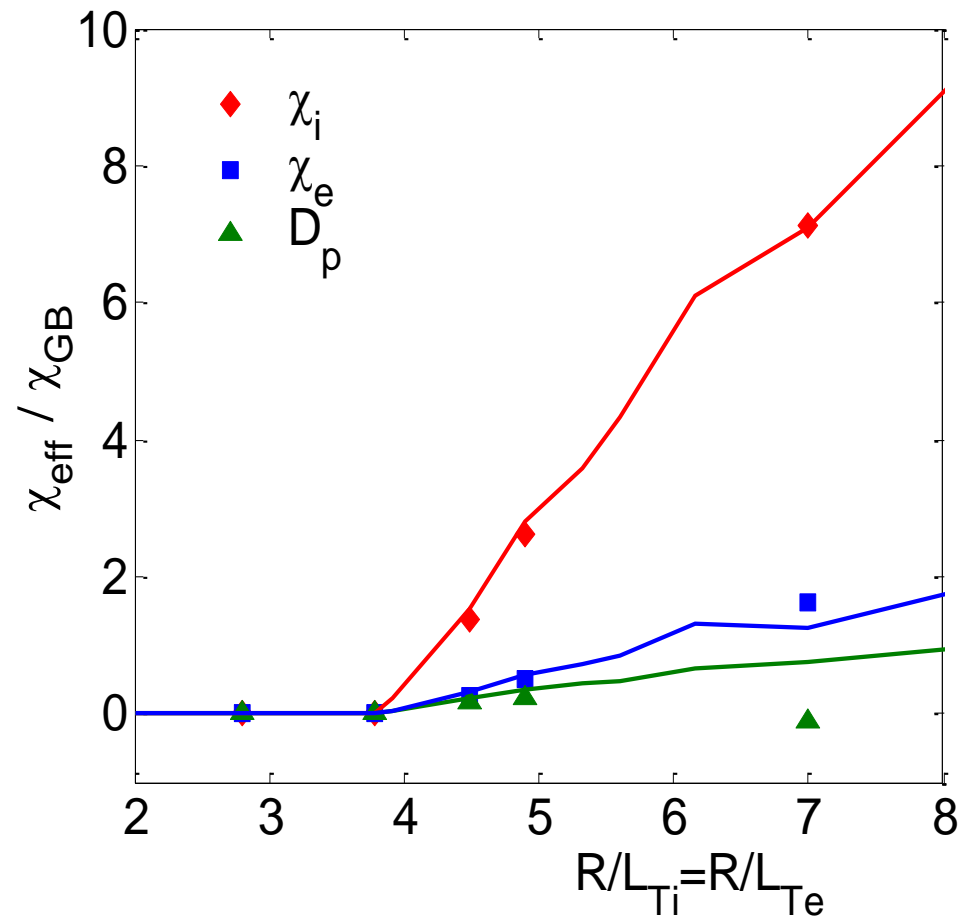
Non-linear GYRO, GENE, GKW (symbols)  
QuaLiKiz (lines)



Quasilinear + other approximations = QuaLiKiz turbulent fluxes  
reproduce well non-linear gyrokinetic fluxes over wide range of parameters  
with computing time  $\sim 30$  s, ready for integrated modeling

Cyclone base case, Dimits PoP2000, with  
kinetic electron  
realistic collisionality

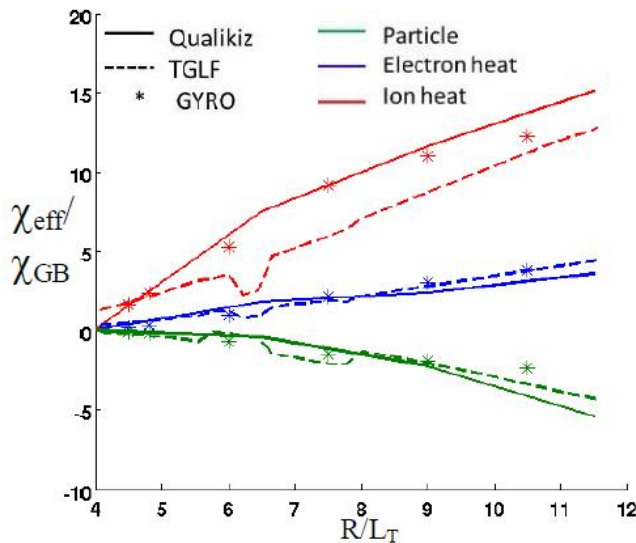
$\rho^*=0.006$ ,  $\beta=0.0$ ,  $v_{ei}[c_s/a]=0.03$   
 $r/a=0.5$ ,  $R/L_{Ti}=R/L_{Te}=7.0$ ,  
 $R/L_n=2.24$ ,  $T_i/T_e=1.0$ ,  $q=1.4$ ,  
 $s=0.78$ ,  $R/a=2.8$



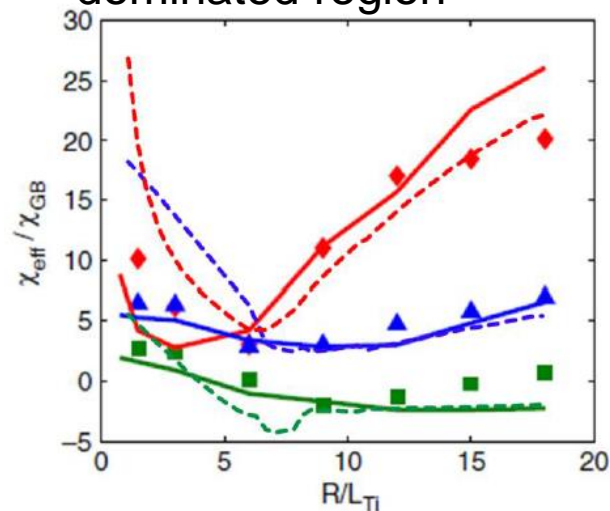
Consistent with high col. kin. EI.  
reduced shift obs. in Mikkelsen, Dorland PRL08

TGLF and QuaLiKiz are accurate enough to be a test of gyro-kinetic theory and are not tuned with experimental data.

- This is not true of other models: Bohm-GB, RLW, CDBM, Coppi-Tang, Multi-mode, GLF23...

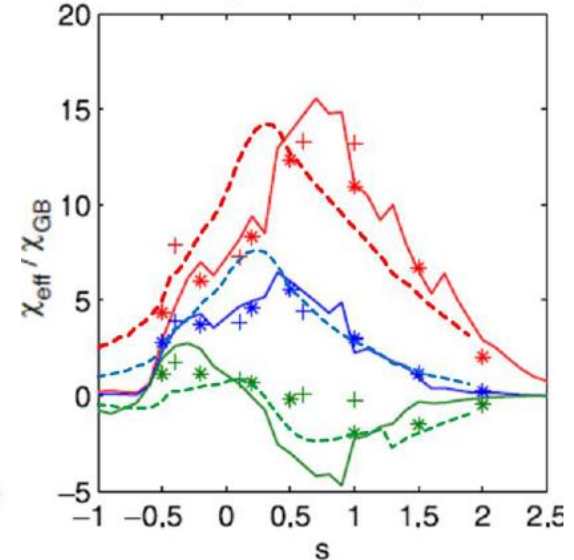


TGLF worse for TEM dominated region



[Staebler ITPA13]

TGLF better for  $s < 0$



[Baicocchi PPCF2015]

	QuaLiKiz	TGLF
Calculated fluxes	Energy, particle and momentum fluxes for unlimited number of ions and electrons	
Dispersion relation	Gyrokinetic  Finds all unstable modes Use the ballooning representation Includes trapped and passing ions and electrons, i.e. ITG-TEM and ETG	Fluid: 12 moments for circulating particles and 3 for trapped  Finds the top two most unstable modes
Eigenfunctions	Estimated in the fluid limit: shifted Gaussians	Hermite basis functions, Gaussian width to maximize $\gamma$ for 1-2 basis functions then refined to 4
Collisions	On electrons, use the Krook operator, energy dependent	On electrons, use a pitch-angle scattering operator, energy dependent
Equilibrium	$s - \alpha$	Bishop eikonal with Miller flux surface shape with elongation, triangularity [40]
Saturated potential: level, $k$ and frequency spectra	Mixing length: $\gamma / \langle k_{\perp}^2 \rangle$ with $k_{\perp}$ accounting for the eigenfunction  $k_{\theta}$ spectrum such that $k_{\theta}^{-3}$ above the maximum and $k_{\theta}$ below  Frequency spectrum: a Lorentzian which width scales as $\gamma$ adjusted for $ s  < 0.6$	Three parameters saturation rule optimized to best fit 160 nonlinear GYRO simulations
$E \times B$	Self-consistently through modified eigenfunctions	Included in spectral shift of saturated potential based on GYRO nonlinear results
Fitted parameters	One, such that, for the GA standard case, QuaLiKiz ion energy flux matches the nonlinear GYRO ion energy flux	All of the parameters were determined by fitting to linear and non-linear theory
Verification	Against nonlinear GYRO, GKW and GENE simulations see table 3	Against 1799 linear gyrokinetic GKS runs and 160 nonlinear GYRO runs

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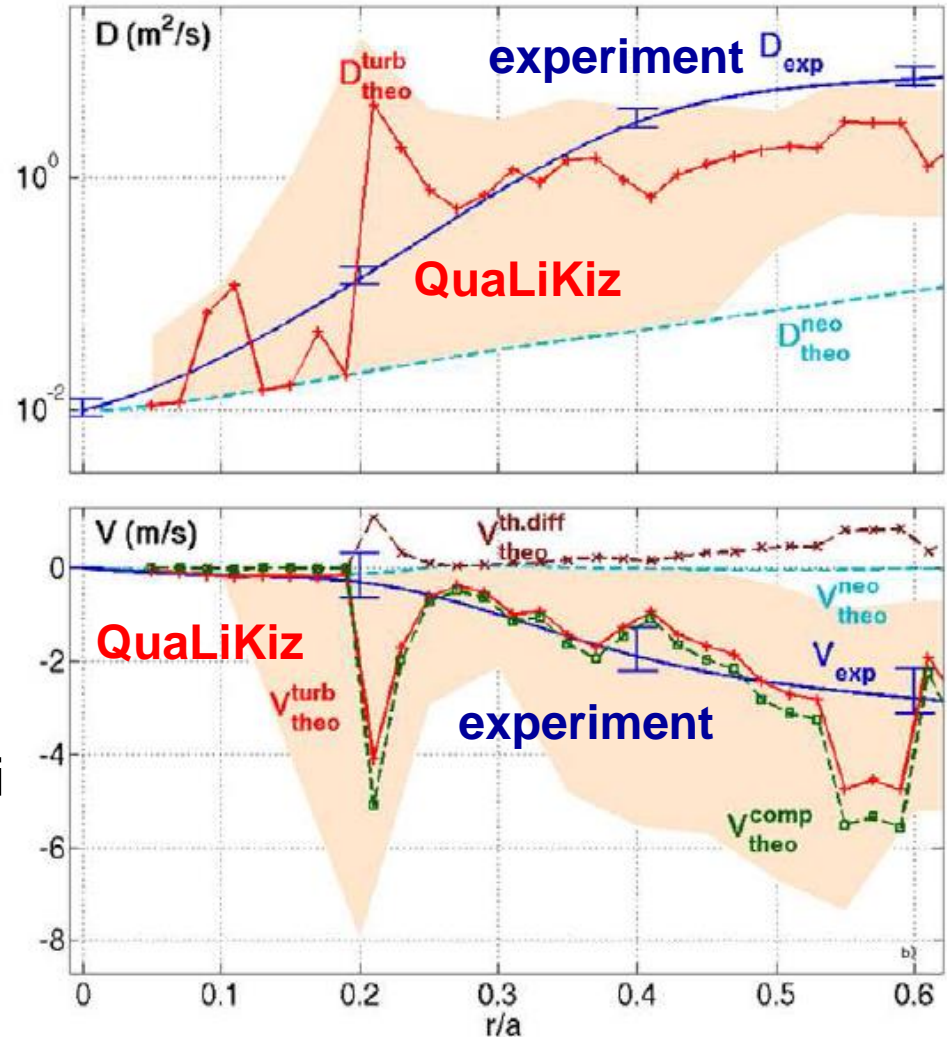
Ni laser blow-off experiments in  
ECRH heated plasmas

$$\Gamma = -D\nabla n + Vn$$

Ni diffusivity increases with  $-\frac{R\nabla T_e}{T_e}$

Convection inward and unsensitive  
to  $-\frac{R\nabla T_e}{T_e}$

Both trends in qualitative and  
quantitative agreement with  
QuaLiKiz diffusive and convective Ni  
flux. Convection dominated by  
compressibility term.





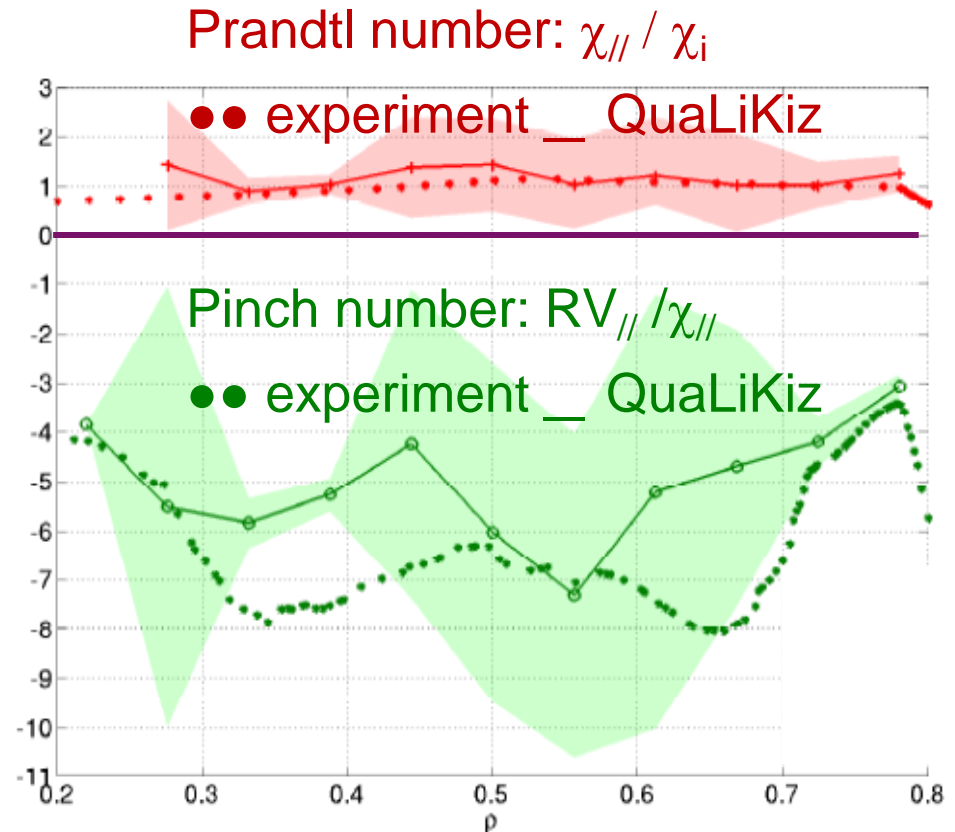
NBI modulation experiment at  
JET [Tala PRL09] proving  
existence of angular momentum  
pinch

**JET**

QuaLiKiz Prandtl number  $\sim 1$   
QuaLiKiz pinch number  $\sim -4 / -7$   
in fair agreement with reported  
experimental values

Fixed gradient approach  
depends on  $\nabla T/T$ ,  $\nabla n/n$ ,  $q$ ,  $s$ ,  
etc lead to large uncertainties  
on prediction

colored regions: **uncertainties** on  $\chi_{//}$  and  
 $V_{\text{pinch}}$  impact of varying within 20%  $U_{//}$ ,  $\nabla U_{//}$   
and  $E \times B$

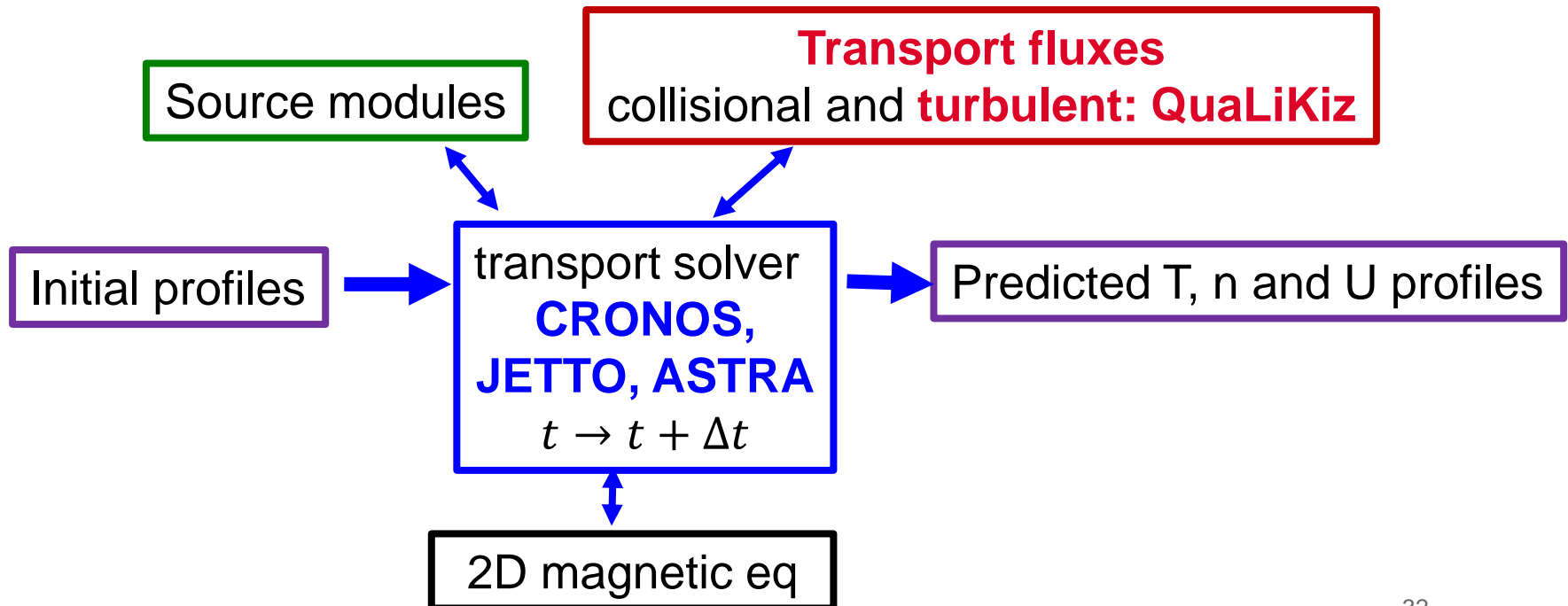


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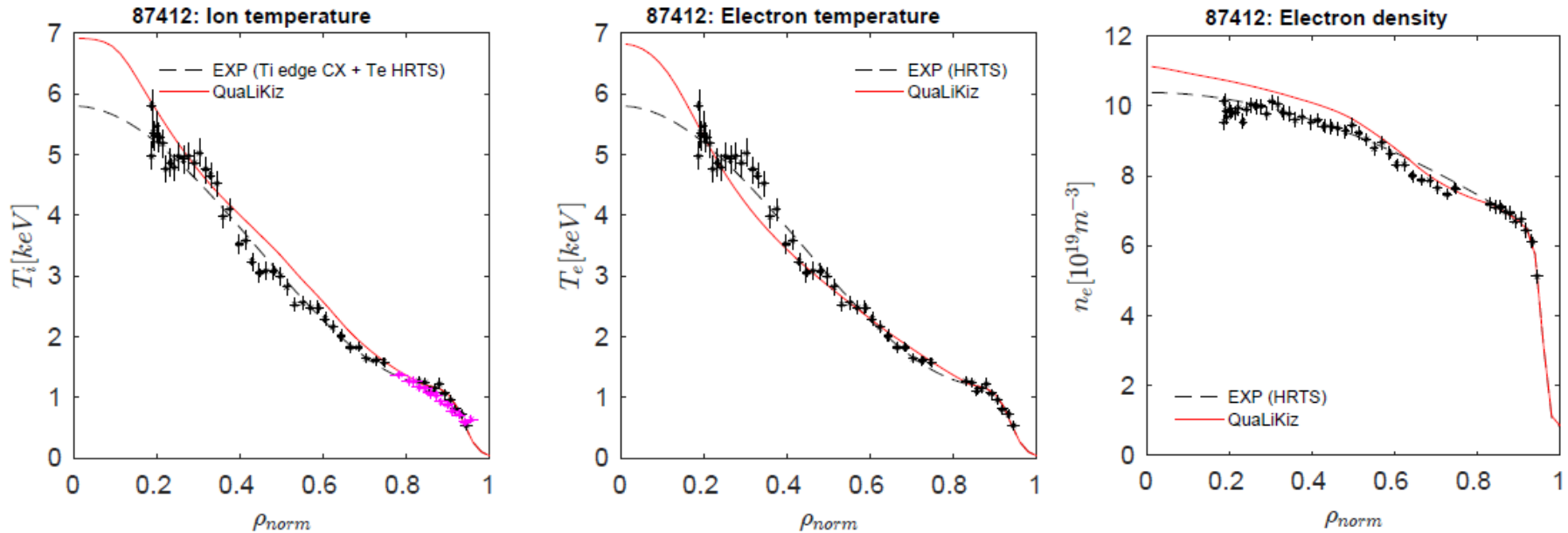
QuaLiKiz turbulent fluxes = Quasilinear + other approximations

$t_{turb.fluxes} < \sim 5 \text{ min}$  for a profile i.e. 20 radial points and 10  $k_{\theta}\rho_s$

- reproduce well non-linear gyrokinetic fluxes over wide range of parameters in  $\sim 10^6$  less computing time
  - in agreement with experimental results at a given time
- ready for integrated modeling



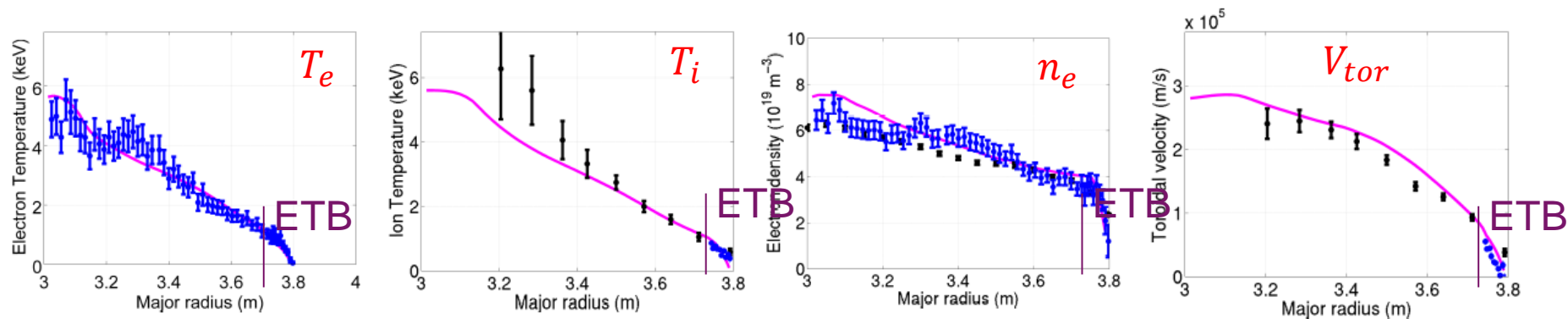
# ILW baseline scenario JET 87412 (3.5MA/3.35T)



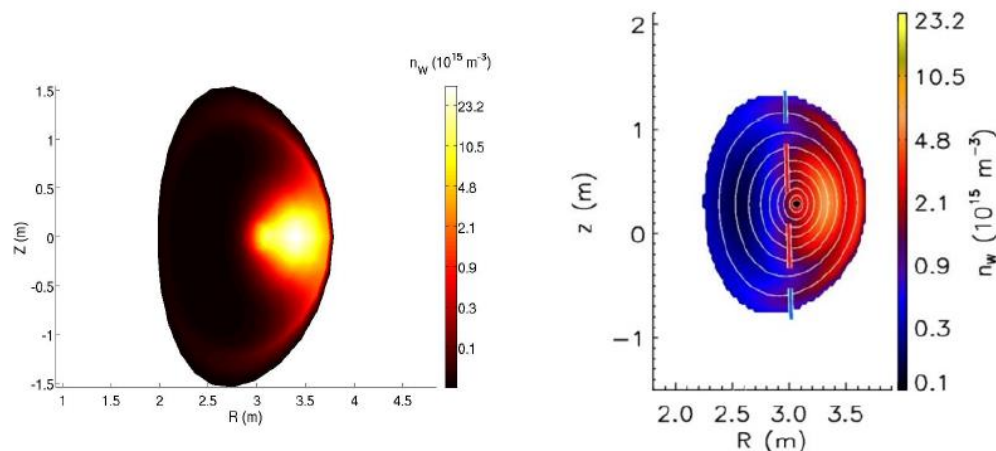
- Boundary condition at  $\rho = 0.85$
- Stable for  $\rho < 0.2$ . No sawtooth model
- Assuming core measurements  $T_i = T_e$  due to poor core CX
- ETG active, leads to  $\sim 10\%$  differences.  $E \times B$  shear stabilization important (not shown due to brevity)

# HYBRID JET-ILW #82722. JETTO-QLK-NEO, INCLUDING W

QuaLiKiz profiles after 1.5 s ( $5x\tau_E$ ) of time evolution



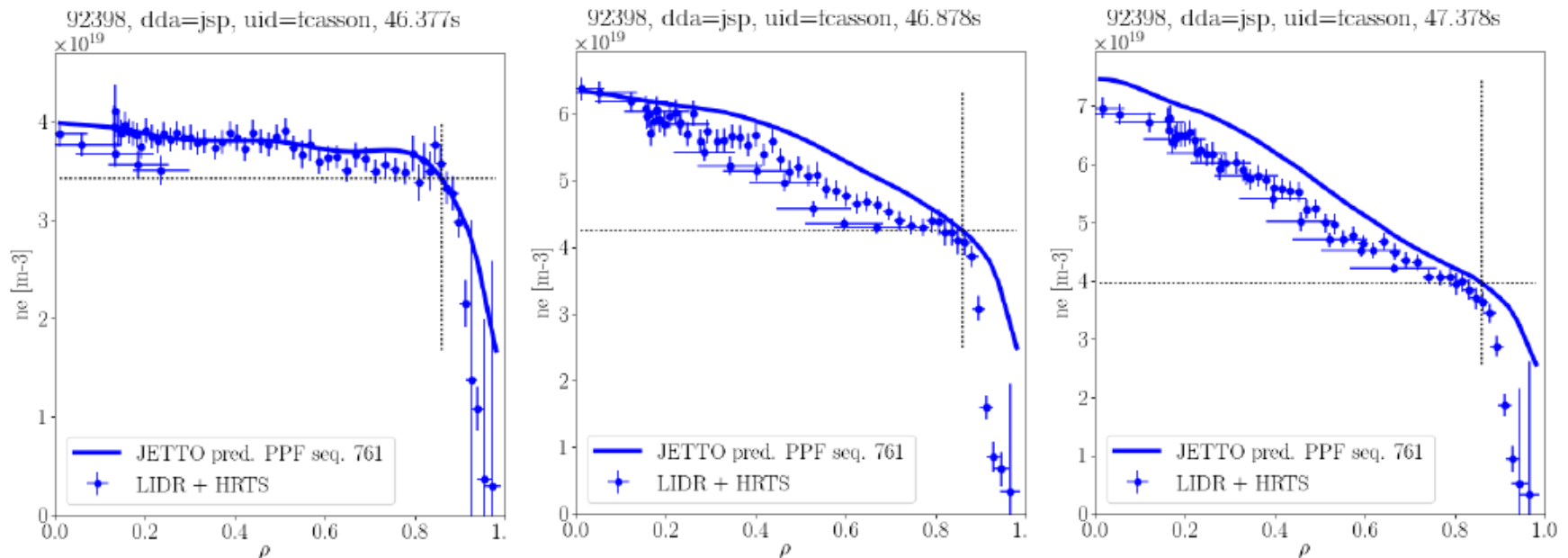
Comparison of  
measured and  
predicted  
2D W-distributions at  
 $t=6.8s$



(a) Predicted  $n_W$  at  $t=6.8s$  after 1.3s of simulation. (b) Experimental estimated  $n_W$  at  $t=6.8s$  after 1.3s of simulation.

# 92398: SECOND HIGHEST PERFORMANCE HYBRID FROM LAST JET CAMPAIGN (C36B)

Density profile time evolution captured, Full line QuaLiKiz



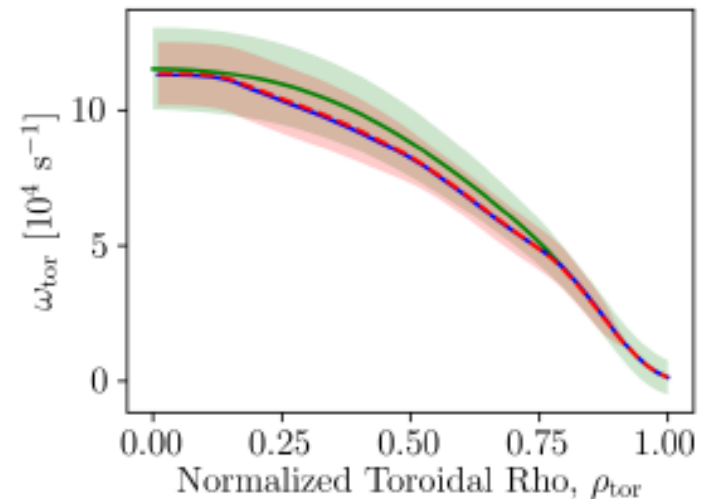
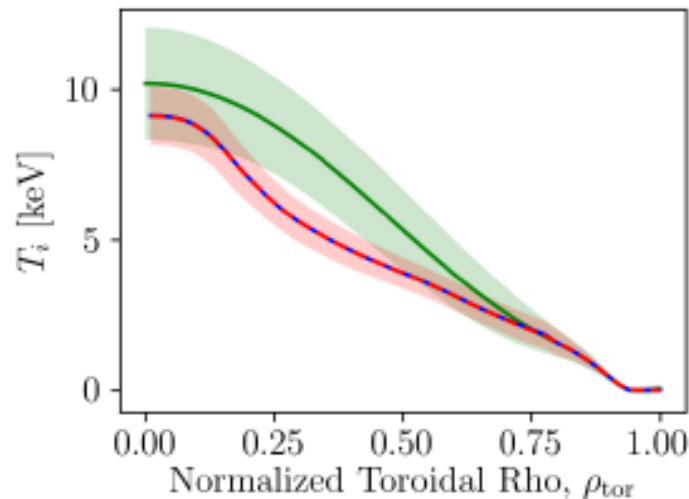
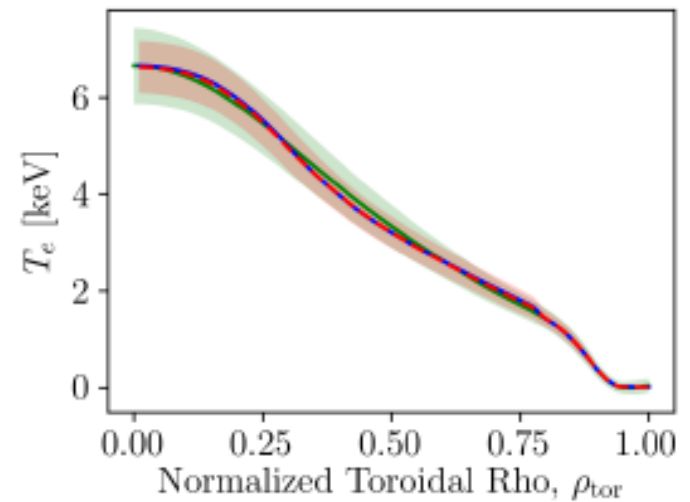
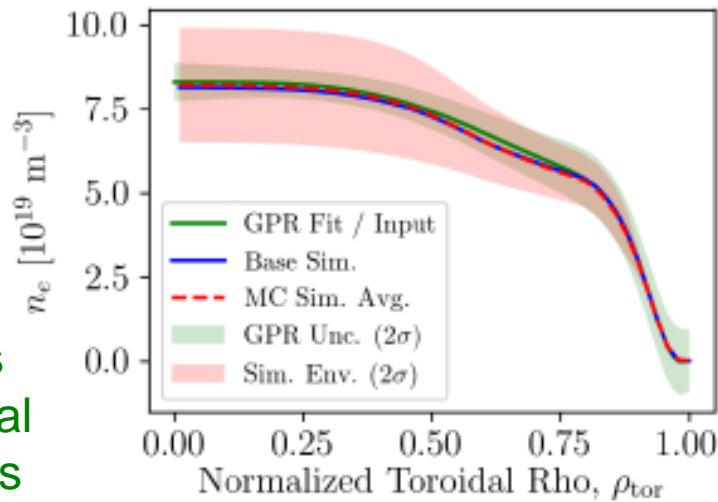
- Fully predictive modelling of high performance hybrid 92398 with JETTO-SANCO-QuaLiKiz-NEO-PION-PENCIL-ESCO
- JETTO-QuaLiKiz fully predictive j,Ni,Ti,Te,Vtor + 3 Imp (including W). 8-channel simulation!
- Motivation: predicting ICRH optimisation for W accumulation control

JET 92436

BC at  $\rho=0.85$

Gaussian  
process  
regression fits  
of experimental  
measurements

JETTO-  
QuaLiKiz,  
Monte Carlo  
sampling of  
input  
boundary  
condition

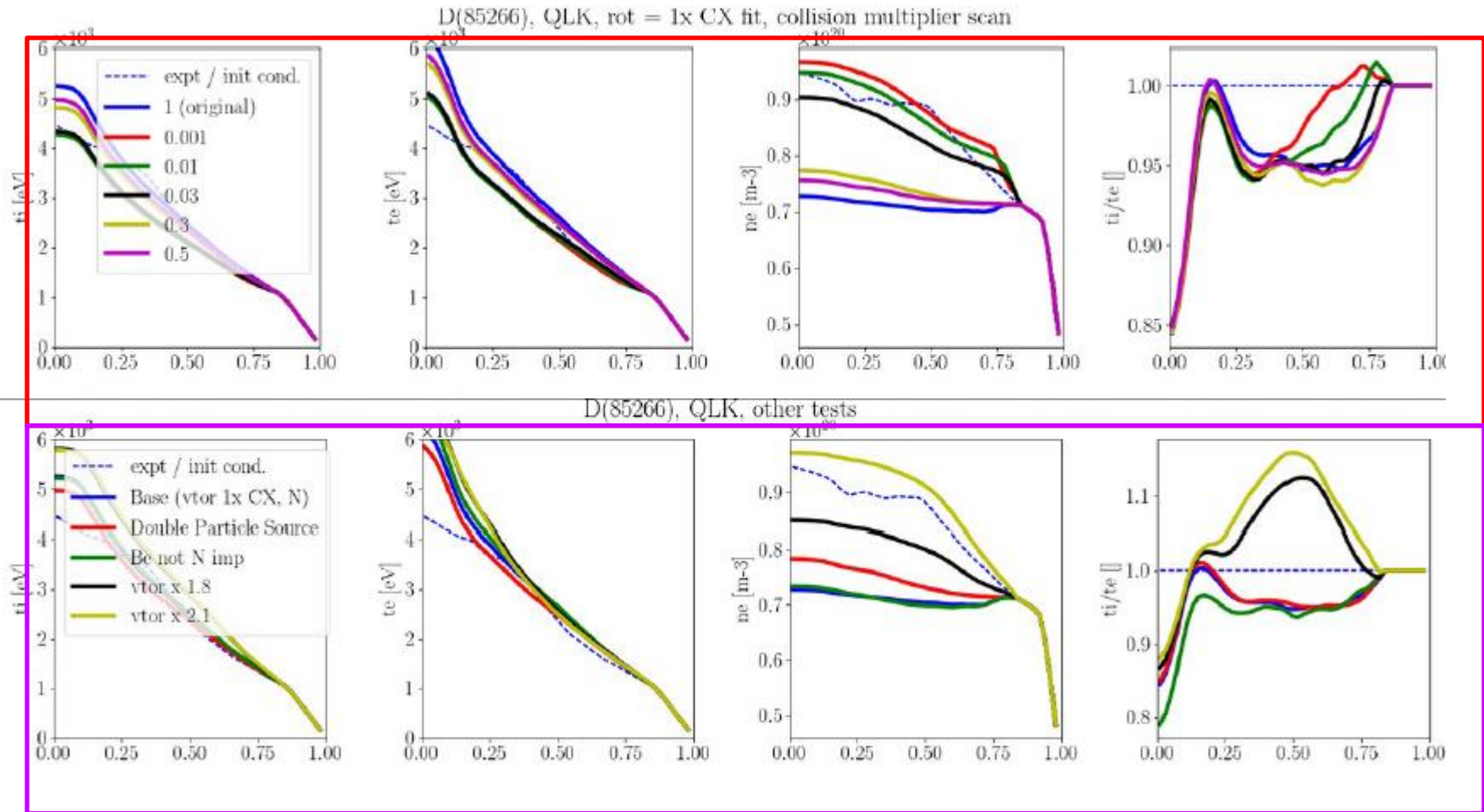


Ti underestimation being investigated

Aaron Ho EPS2017, paper in prep.



Too flat density for an L mode case (courtesy T Bache and FJ Casson)  
Peaking recovered by artificially **reducing collisions** or **increasing Vtor**



- Linear gyrokinetic formulation
- Linear stability and experimental observations
- Deriving and validating quasilinear particle, momentum and heat fluxes
- Quasilinear fluxes vs experimental observations
- Towards density, temperature and rotation profiles prediction
- Conclusions and perspectives

- The quasilinear approximation is valid in a wide range of parameters, extensively checked [Casati 2009, Citrin 2012, Angioni's, Jenko's work (see ref in Casati 2009 for example)]
- 2 existing quasilinear codes that are CPU compatible with integrated modelling needs: QuaLiKiz [us] and TGLF [Staebler, Waltz, Kinsey GA, USA]
- Successful multi channels and multiple confinement time predictions by quasilinear codes [Citrin PPCF2017, Breton to be submitted, Linder on AUG to be submitted, Casson on-going]
- But....

- **In integrated modeling framework:**
  - Understand the cause of the overestimated density profile flattening in some L mode cases
  - Is the LOC-SOC transition reproduced? [Bourdelle EPS2017, on-going]
- **In stand alone framework:**
  - $s$ - $\alpha$  interchange modes stabilization overestimated in QuaLiKiz vs GENE [Linder internship report 2016] pb for steady-state regimes with flat and reversed q profiles (ITB) [Citrin PPCF 2017]
  - W turbulent transport: impact of trace assumption for poloidal asym. At which level of W concentration the assumption fails (QuaLiKiz vs GWK) [Citrin PPCF 2017]
  - roto-diffusion forced to 0 because strange behavior: significative for heavy ions nonetheless. Need to understand pb [Citrin PPCF 2017]
  - Add Impact of elongation (K), test Weiland's  $\hat{s} = \sqrt{2s-1} + K^2(s-1)^2$  on R/Ln, R/LT values vs GENE/GWK

[www.qualikiz.com](http://www.qualikiz.com)

**Open source code, available on GitHub.**

- **Links to key publications**, where the detailed QuaLiKiz derivation can be found
- **all above issues in « issue tracker »**, and anyone should **open an issue tracker whenever encountering a bug or strange behaviour related to QuaLiKiz**
- **All published integrated modeling runs to be archived and documented** also on this page whether JETTO/ASTRA/CRONOS/METIS/RAPTOR. 1st level table being prepared.

JETTO-QuaLiKiz info is available on JETTO wiki pages:

[https://users.euro-fusion.org/tfwiki/index.php/JETTO\\_Qualikiz](https://users.euro-fusion.org/tfwiki/index.php/JETTO_Qualikiz)

Will be improved further soon.

And also there, a table with catalogued published JETTO-QuaLiKiz cases has to be made for all users