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Predict First: flux-driven multi-channel integrated modelling over multiple confinement times with the gyrokinetic turbulent transport model QuaLiKiz

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JET

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Dutch Institute for
Fundamental Energy Research

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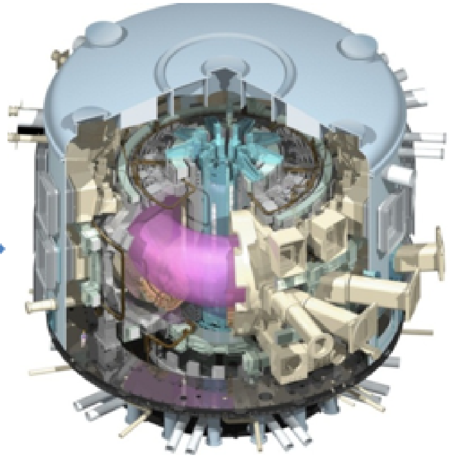
Motivation: integrated tokamak modelling demands tractable calculations of all components

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

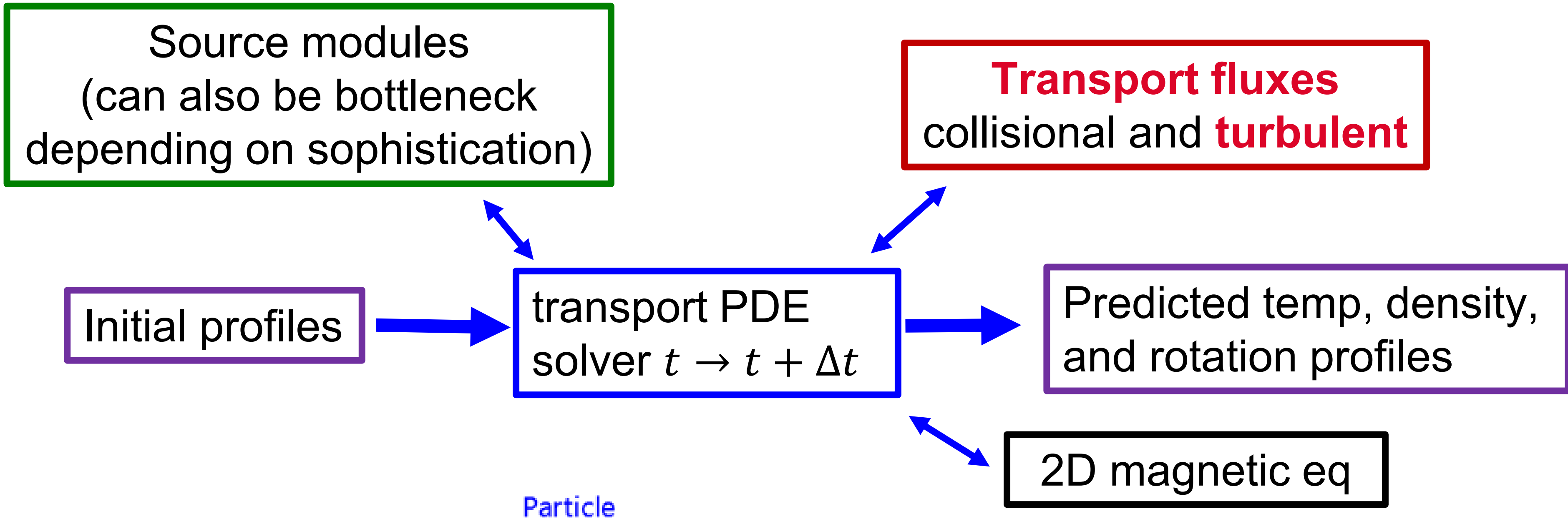
- Magnetic equilibrium
- Heating
- MHD stability
- Turbulence
- Plasma-wall-interaction



- Fusion power
- Heat exhaust

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

Turbulence typically bottleneck in core transport modelling: demands multiple calls for profile dynamics



Source modules (can also be bottleneck depending on sophistication)

Transport fluxes collisional and **turbulent**

Initial profiles

transport PDE solver $t \rightarrow t + \Delta t$

Predicted temp, density, and rotation profiles

2D magnetic eq

Particle flux

Particle sources/sinks

Particle density: $$\frac{\partial n_s}{\partial t} + \frac{1}{r}\frac{\partial}{\partial r}(r\Gamma_s) = S_s$$

Energy: $$\frac{3}{2}\frac{\partial P_s}{\partial t} + \frac{1}{r}\frac{\partial}{\partial r}(rq_s) = Q_s$$

Heat flux

Heat sources/sinks

Typical solver timestep $\Delta t \approx 1ms$

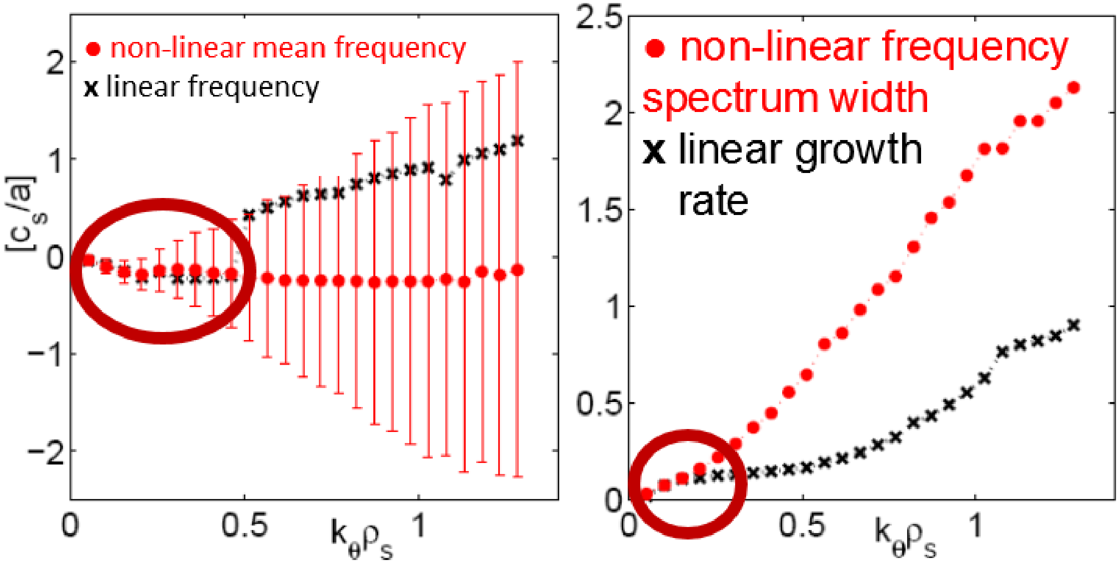
$O(10^4)$ turbulence model calls during a full tokamak simulation.

Profile dynamics challenging with nonlinear gyrokinetics:$> 10^4$ CPUh per call, $>10^8$ CPUh total

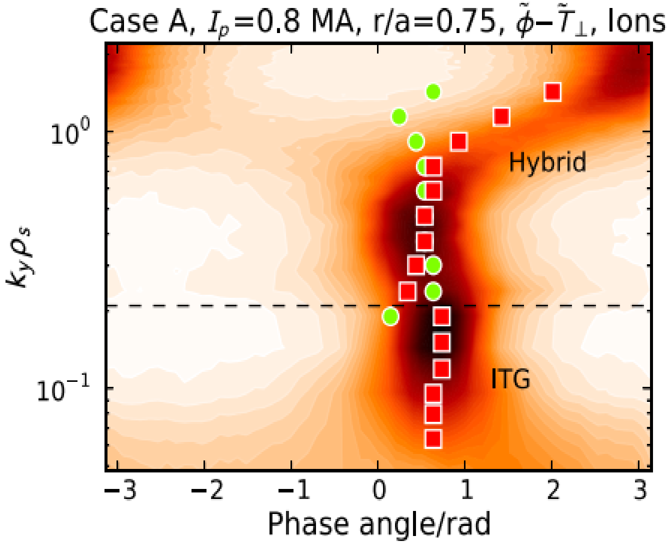
"Quasilinear" transport models provides shortcut in wide regimes: assumptions justified by nonlinear simulations

1. Well known that in tokamak core ($\rho_{norm} < 0.9$) fluctuations are small, O(1%)
2. Nonlinear simulations show strong signatures of underlying linear modes at transport driving wavenumbers ($<0.5\ k_\theta \rho_s$). Mean frequency, frequency broadening, and phase-shift matching. Supports applying linear response for transport estimates

GYRO linear and non-linear of
Tore-Supra 39596 at r/a = 0.7 [Casati 2009 PhD]



GENE linear and non-linear $\delta\phi - \delta T_\perp$ phase shifts in AUG case (Told PoP 2013)



See also: Dannert PoP05, Lin PRL07, Merz PRL08, Casati NF09, Citrin PoP 2012

QuaLiKiz: a quasilinear gyrokinetic transport model $\times\, 10^6$ faster than local δf gyrokinetics

Dispersion relation: linearised electrostatic Vlasov equation + quasineutrality (weak form). $\hat{s}-\alpha$ geometry

Local plasma parameters reflected in following terms

ω^* : diamagnetic frequency (driving terms)

$k_\parallel v_\parallel$: parallel dynamics (=0 for bounce averaged trapped species)

ω_D : ∇B-curv drift (perpendicular dynamics)

ν : collisionality (kept only for trapped electrons)

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

$\delta\phi$ eigenfunction solved from high ω expansion of D(ω) and shifted-Gaussian ansatz (symmetry breaking with rotation). Further $O(10^{2-3})$ speedup compared to standard linear gyrokinetics

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

$\sim$1 CPU second to solve for each wavenumber (n). ITG, TEM, and ETG modes

Quasilinear fluxes for heat, particle, momentum transport with nonlinear saturation rule

Transport fluxes for species j: carried by $E \times B$ radial drifts

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

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 is the "saturation rule" validated by turbulence mesasurements and nonlinear simulations (see Casati PRL '09, NF '09, Citrin PoP 2012, PPCF 2017).

For more details: Bourdelle PPCF 2016, Citrin PPCF 2017, Stephens arxiv.org/abs/2103.10569 and www.qualikiz.com (open source on GitLab)

- Transport assumed local! Relative impact of nonlocal effects an open research question
- No Dimits shift! (although reduced to <15% in kinetic electrons ES NL simulations, Mikkelsen PRL 2008)

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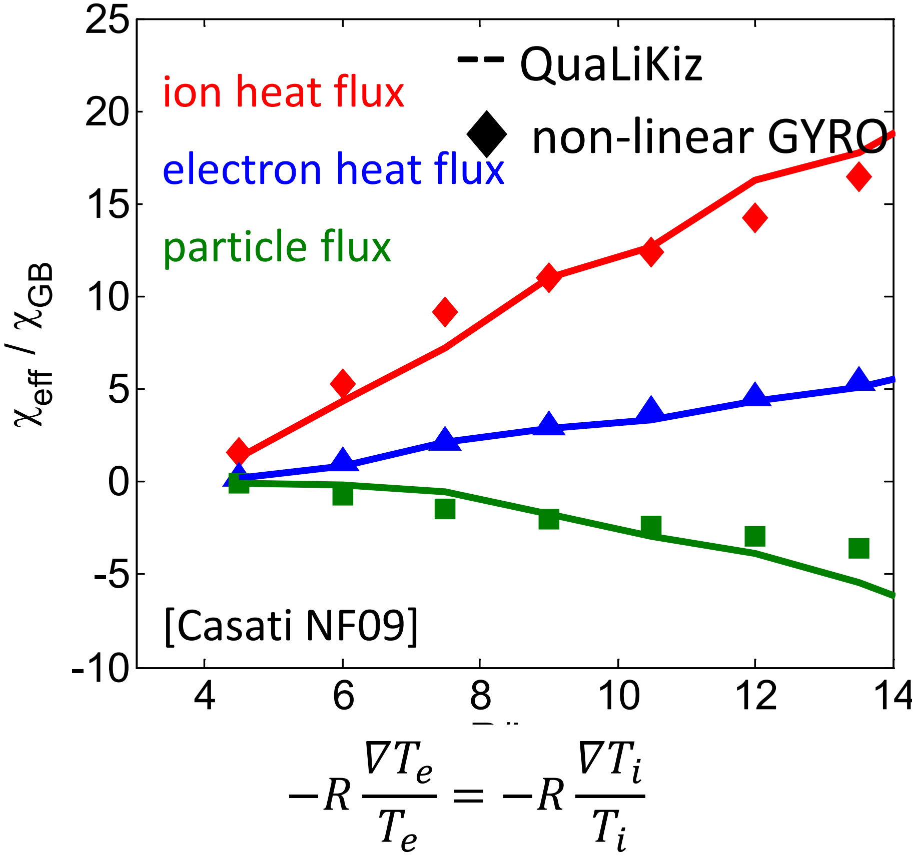
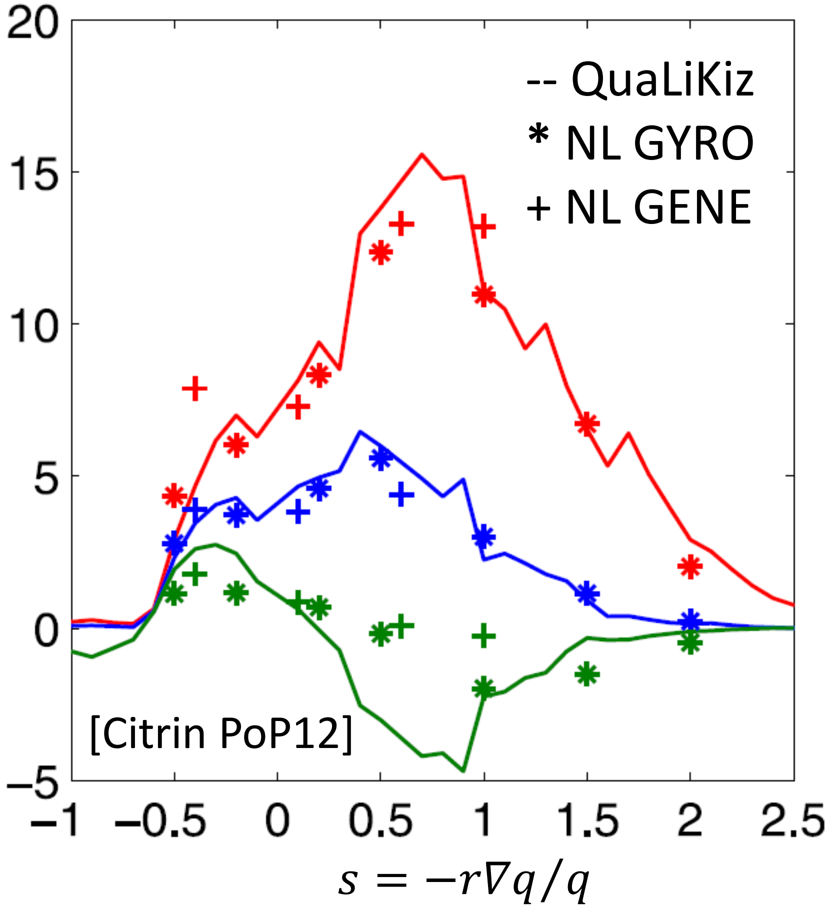
QuaLiKiz reproduces non-linear fluxes over wide range of parameters, but × 10^6 faster

Parameter scans around GA-Standard case

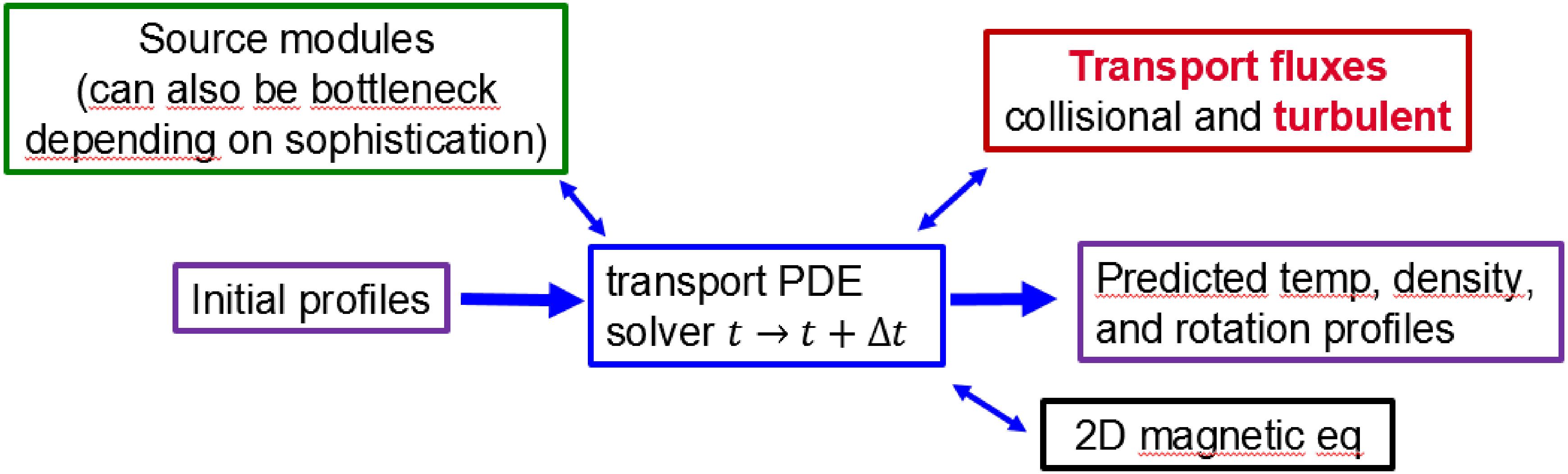




Continuous process of nonlinear verification and experimental validation of QuaLiKiz, identifying parameter regimes for model improvement

Extensive QuaLiKiz validation and physics studies recently achieved within integrated modelling

- Speed-optimized QuaLiKiz (Citrin PPCF 2017) in JINTRAC [1,2] and ASTRA [3] for integrated modelling
- This talk focuses on validation against JET discharges. Successful validation for AUG [O. Linder Nucl. Fusion 2018, P. Manas *to be submitted*] and WEST [P. Maget *to be submitted*] as long as regime is not TEM dominated
- ~100CPUh for 1s of JET plasma. Efficient parallelization to ~20 cores. Subsequent simulations are with JINTRAC



Source modules
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Initial profiles

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solver $t \rightarrow t + \Delta t$

Predicted temp, density,
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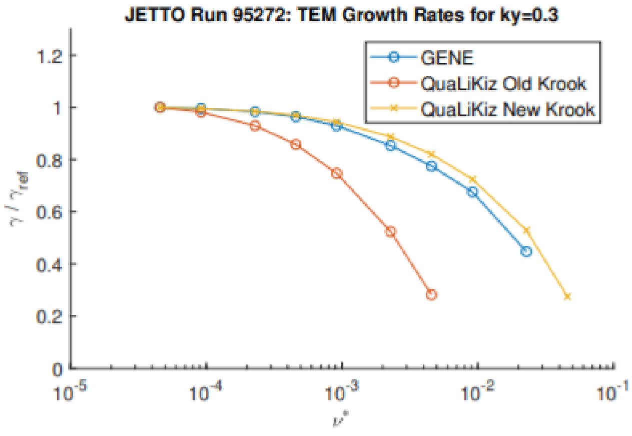
2D magnetic eq

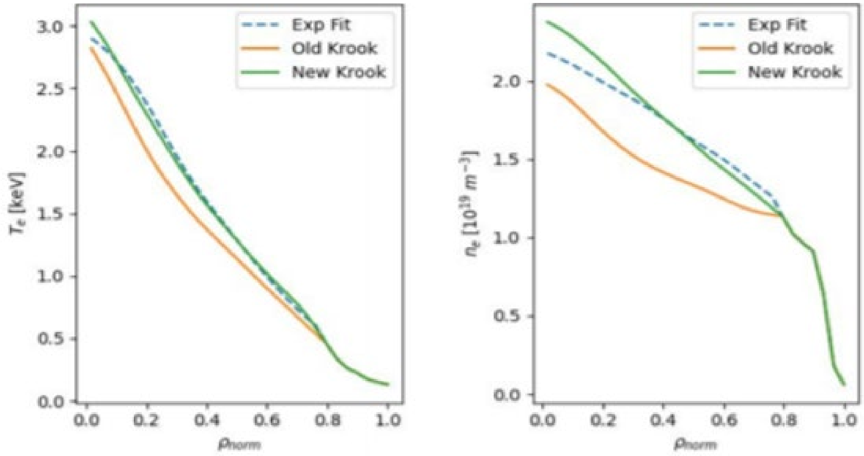
[1] G. Cenacchi, A. Taroni, JETTO: A free-boundary plasma transport code, JET-IR (1988)
[2] M. Romanelli 2014, Plasma and Fusion research 9, 3403023-3403023
[3] G.V. Pereverzev and Y.P. Yushmanov. ASTRA Automated System for Transport Analysis in a tokamak . IPP - Technical Report, (5/42), 2002

Most recent release QuaLiKiz 2.8.1 has improved numerics and an improved Krook-like collision operator

Re-calibration of QuaLiKiz Krook-like collision operator against GENE collisionality scans [C. Stephens, *to be submitted*]. Triggered by QuaLiKiz flat-density predictions in mid and high collisionality regimes


JETTO Run 95272: TEM Growth Rates for ky=0.3

JET 79815



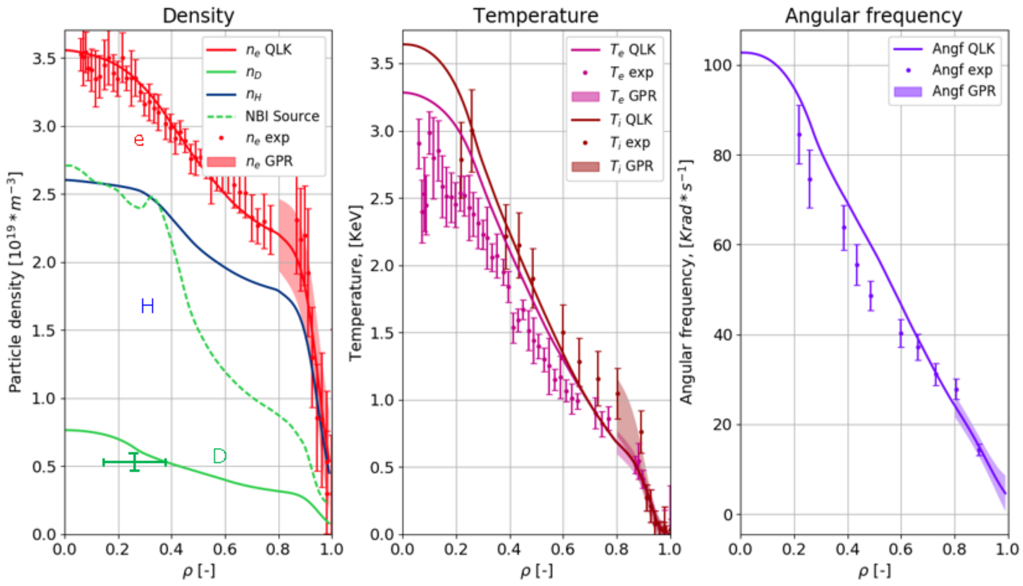
Significantly improved QuaLiKiz model validation on JET H-mode and L-mode collisionality scans from T. Tala NF 2019.

QuaLiKiz 2.8.1 also includes an open source replacement for proprietary NAG cubature. New cubature routines more robust, and up to factor 2 faster. QuaLiKiz now fully open source (qualikiz.com)

A limited selection of recent JINTRAC-QuaLiKiz validation studies on JET discharges

Multiple-isotope predictions show weak isotope dependence on source and fast isotope mixing as seen in experiments

JET-ILW 91232 with H-D mix. Core particle source was purely D



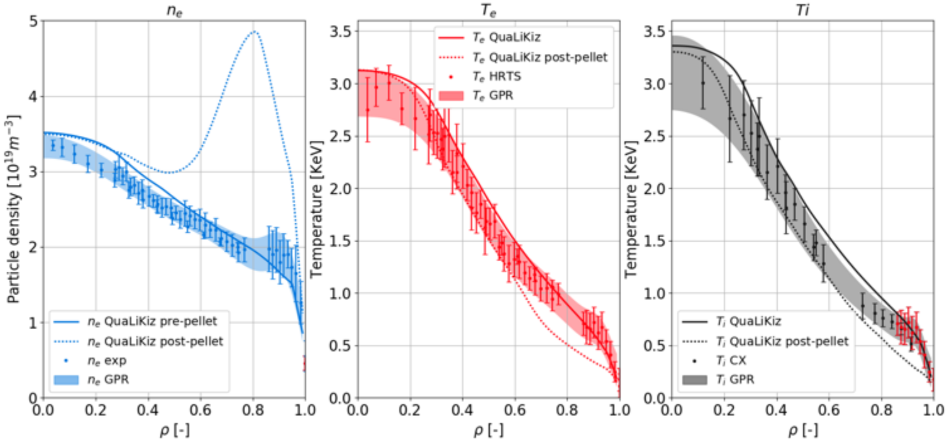
- Fast transport of ions and isotope peaking with no core source seen experimentally and understood as natural consequence of ITG regime [Maslov NF 2018, Bourdelle NF 2018]
- Peaked H profiles with no core H source predicted by JETTO-QuaLiKiz in agreement with multiple isotope experiments
- Validation of T_e, T_i, n_e, v_{tor} predictions. Inner core n_D in agreement with neutron inferrence

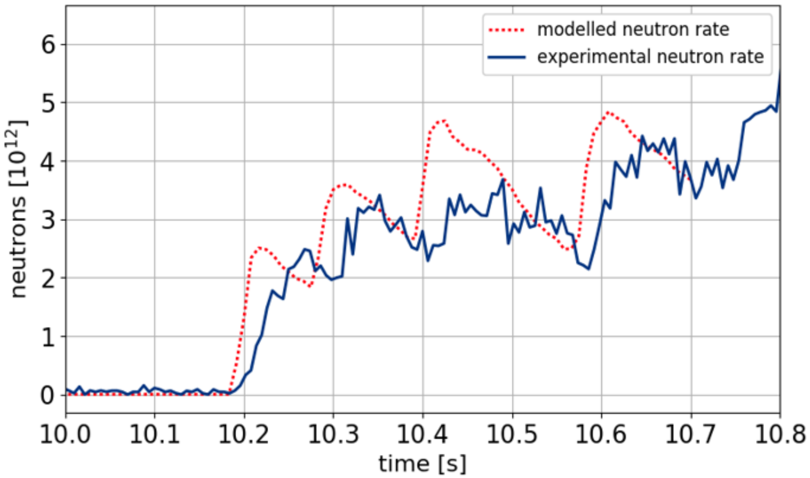
Concomitant prediction of fast mixing of isotopes during transients (e.g. pellets).

Positive ramifications on DT mix control and He ash removal if reactor in ITG or mixed ITG-TEM regime

M Marin Nucl. Fusion 2020

Fast deuterium penetration in JET mixed isotope plasma pellet fuelling experiment is reproduced by JINTRAC-QuaLiKiz





- JET experiment: D pellets in H plasmas. Pre-pellet H-plasma. Neutron rate measures fast D penetration [Valovic NF 2020]
- JINTRAC-QuaLiKiz core modelling (boundary condition $\rho = 0.9$) with HPI2 pellet model
- Good reproduction of pre-pellet T_i, T_e, n_e
- Following pellet ablation, for $\rho < 0.8$, strong negative R/L_{ne} forms (stabilizing), but compensated by increasing R/L_T due to local cooling. ITG remains unstable. Mechanism validated vs linear and nonlinear GENE
- Ion transport coefficients are large for ITG turbulence, allows fast deuterium penetration on energy confinement timescale, in agreement with neutron measurements

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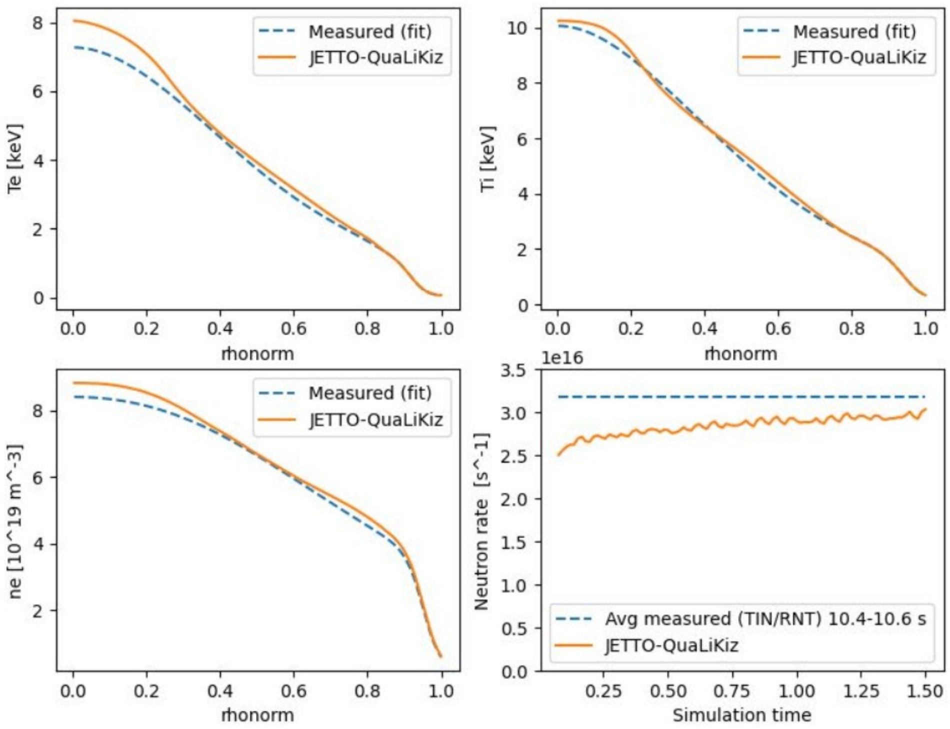
M Marin Nucl. Fusion 2021, and this conference

QuaLiKiz validated against JET high performance baseline and hybrid scenarios, subject to DT extrapolation

96994: fits avgd 10.4-10.6 s	**Baseline scenario 3MA/2.8T (q_{95}=3.1) ~32MW heating**
Boundary condition	rho=0.85. Fixed based on fit average between 10.4-10.6 s
Simulation time	1.5 seconds (until stationary state)
Predicted profiles	q, Te, Ti, ne
Impurities and radiation	Prescribed Be, Ni, N, W inferred via Sertoli method [M. Sertoli JPP 2019]
NBI	PENCIL predicted, voltage/power: 112.5kV/12MW (4) ; 118kV/16.25MW (8)
ICRH	PION predicted, input power = 3.5MW, freq = 42.5MHz, 3% H
Turbulent transport	QuaLiKiz 2.8.1 Ad-hoc EM stabilisation [Casson NF 2020]. Prescribed transport patch for rho < 0.2
Initial q + Equilibrium	Initial condition from kinetic constrained EFIT Self-consistent evolution with ESCO



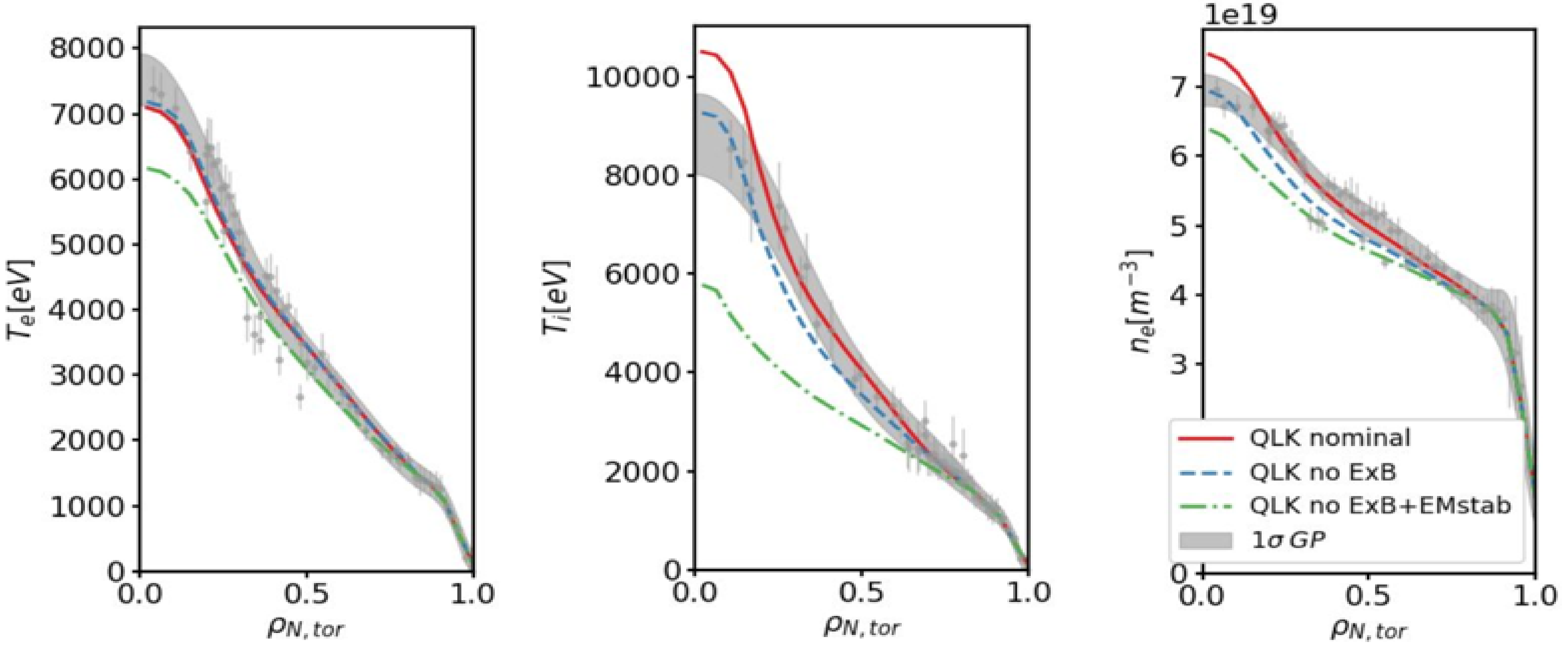
- Good reproduction. Neutrons within ~10% of measured
- Only modification was n_e boundary condition $\times 1.05$
- Similar results for JET high performance hybrid scenario, omitted for brevity
- Extrapolation to DT consistent with JET targets *(see J. Garcia, this conference)*

H.T. Kim, J. Citrin, M. Marin, and JET T17-07 DT extrapolation task team

High performance JET scenarios well predicted by QuaLiKiz. Caveat: EM-stabilization of ITG captured by ad-hoc model

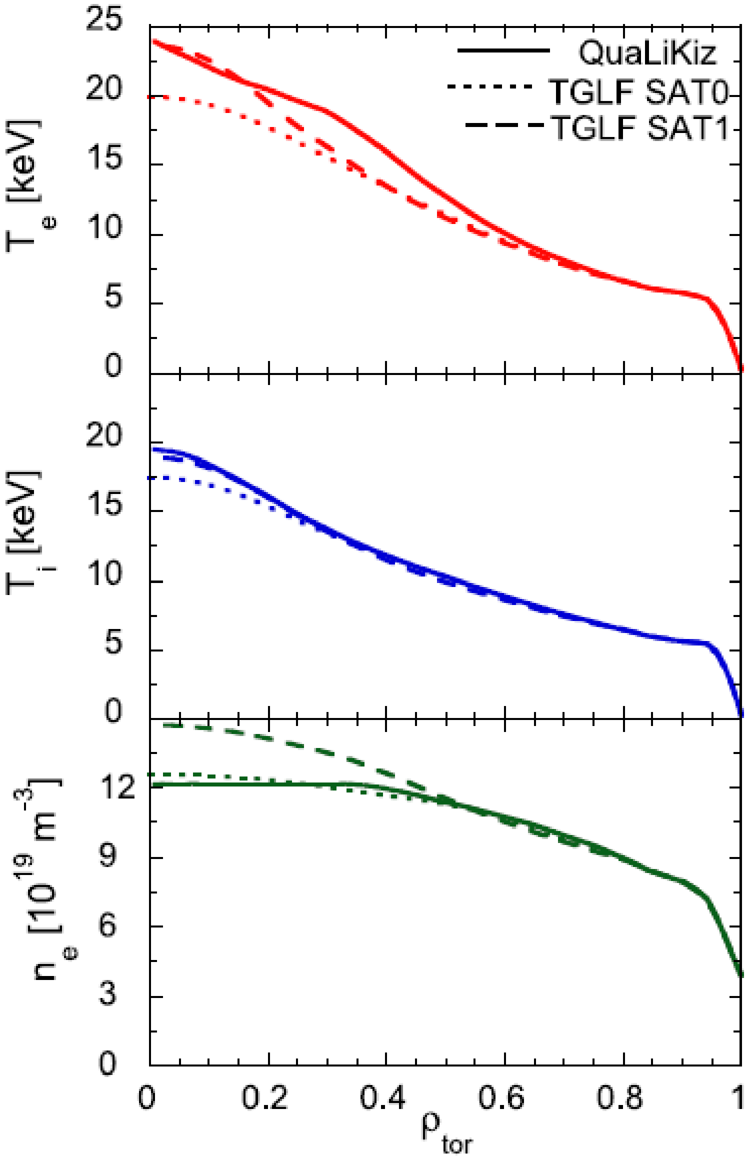
JET high performance hybrid scenario #94875

$I_p = 2.8\,MA, B_T = 2.2\,T, H_{98} = 1.2, \beta_N = 2.34$



- Both $E \times B$ shear and EM-stabilisation important for high-performance accurate prediction
- Caveat! EM-stabilization of ITG, including fast ions [Citrin PRL 2013, PPCF 2015, Doerk NF 2017, di Siena NF 2020], not predicted by first-principles in QuaLiKiz. Employs ad-hoc correction to R/L_{Ti} [Casson NF 2020]. Expansion of QuaLiKiz to include electromagnetic effects is desirable

JINTRAC-QuaLiKiz extrapolations to ITER baseline $I_p = 15MA$ scenario predict $Q \sim 10$ in line with targets



- EPED consistent pedestal pressure boundary condition of 130 kPa
- Heat and particle transport predicted
- $P_{fus} \sim 510\ MW,\ Q \sim 9.5$
- Similar predictions for both QuaLiKiz and TGLF

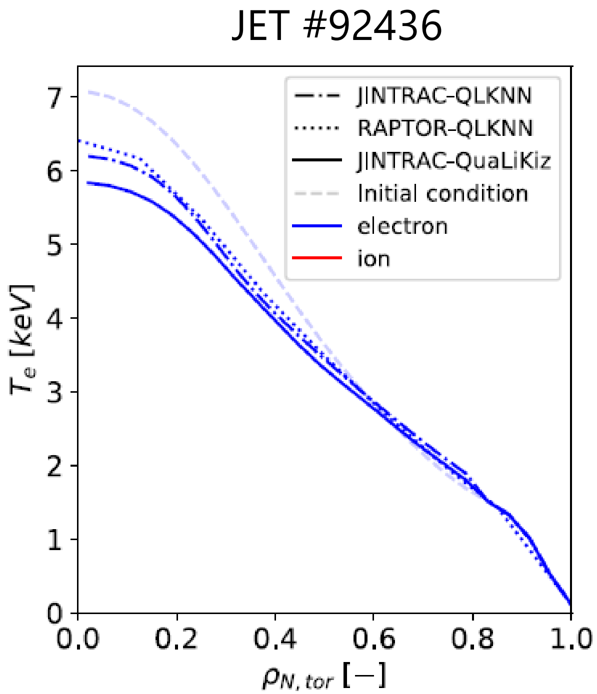
P. Mantica PPCF 2020

QuaLiKiz neural network surrogate model trained on HPC-generated database applicable for optimization, control, and experimental design

$3 \cdot 10^8$ QuaLiKiz turbulence calculations with 1.5 MCPUh on Edison@NERSC. 9D input lattice for generality

Quantity	Range	# points
Wavenumbers (ion + electron scale) [$k_\theta \rho_s$]	0.1 – 36	18
Ion temperature gradient [R/L_{T_i}]	0 – 14	12
Electron temperature gradient [R/L_{T_e}]	0 – 14	12
Density gradient [$R/L_{n_e} (\equiv R/L_{n_i})$]	-5 – 6	12
Magnetic pitch angle [q]	0.66 – 15	10
Magnetic pitch angle shear [$\hat{s}$]	-1 – 5	10
Normalized radius [r/R]	0.03 – 0.33	8
Temperature ratio [T_i/T_e]	0.25 – 2.5	7
Collisionality [ν^*]	10^{-5} – 1	6
Impurity content [Z_{eff}]	1 – 3	5

Impact of $E \times B$ shear included in post-processing


JET #92436

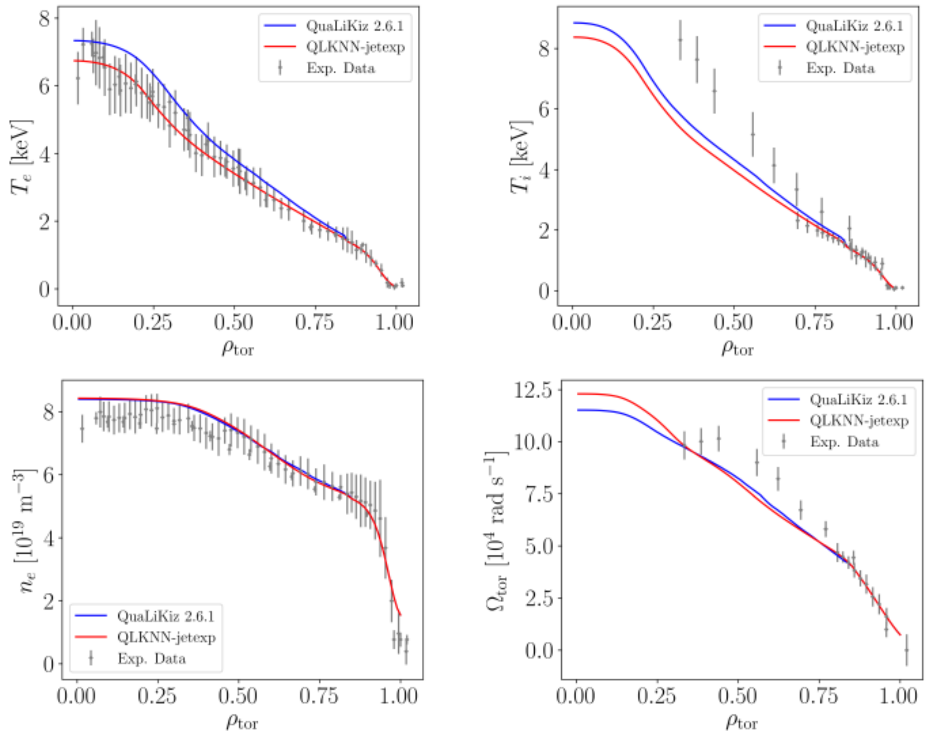
QLKNN-hyper-10D coupled and benchmark on JINTRAC and RAPTOR

- Feed-forward-neutral-network (NN) regression of QuaLiKiz database reproduces accurately the QuaLiKiz input-output structure. Physics-informed methodology is key
- QuaLiKiz-neural-network (QLKNN) applicable as a fast surrogate transport model. QLKNN evaluation is $\times 10^5$ faster than QuaLiKiz. Provides transport flux profiles in <1ms

K.L van de Plassche PoP 2020

QLKNN-jetexp-15D: a QLKNN variant with more input dimensions for higher fidelity, constrained to JET dimensionless parameter space

JET baseline #92436



- Training set for QuaLiKiz neural network sampled from multiple time windows from 2145 JET discharges (based on JETPEAK)
- Training set varied T, n, v_{tor} gradients based on error bars of Gaussian Process Regression fits [Ho NF 2019]. $\sim 20M$ I/O sets
- Validated against full-QuaLiKiz and range of JET experiments in multiple regimes
- Now in production mode. Early promising applications under way for hybrid scenario ramp-up optimization
- Fast! JINTRAC-QuaLiKiz: ~3 days on 16 cores
  QLKNN-jetexp-15D: ~2 hours on 1 core
  (and turbulent transport no longer bottleneck)

A. Ho PoP 2021

Summary and outlook

- Quasilinear turbulent transport assumptions justified through verification and validation
- QuaLiKiz: gyrokinetic quasilinear transport model. $\times\, 10^6$ faster than δf local nonlinear GK.
- Key advantage is to study dynamic interaction of multiple transport channels, sources and sinks
- Neural network surrogate of QuaLiKiz additional $\times\, 10^5$ speedup. Exciting avenues for scenario development and control-oriented simulation.
- Ongoing work to further validate and improve the QuaLiKiz model. Present challenges include: TEM-dominated regimes, EM-effects from first-principles, impurity transport, shaped geometry

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QuaLiKiz is open source, new users welcome: **www.qualikiz.com**
Overview papers: [Bourdelle PPCF 2016, Citrin PPCF 2017, Stephens JPP submitted]

Join the team!

- QuaLiKiz development: C Bourdelle, J Citrin, C D Stephens, X Garbet,
  K.L. van de Plassche, F. Jenko, et al

- QuaLiKiz integrated modelling:
  - using JINTRAC: F J Casson, C Bourdelle, J Citrin, A Ho, M Marin, I Casiraghi, et al…
  - using ASTRA: P Manas, E Fable, et al …
  - using RAPTOR (QLKNN): P Manas, F Felici, S van Mulders, et al…

- QuaLiKiz neural network:
  K. L van de Plassche, A Ho, J. Citrin, C. Bourdelle, Y. Camenen, F. Felici, et al…

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