

Advanced transport models for energetic particles

20th European Fusion Theory Conference, 2.-5. October 2023, Padova, Italy

ATEP team:

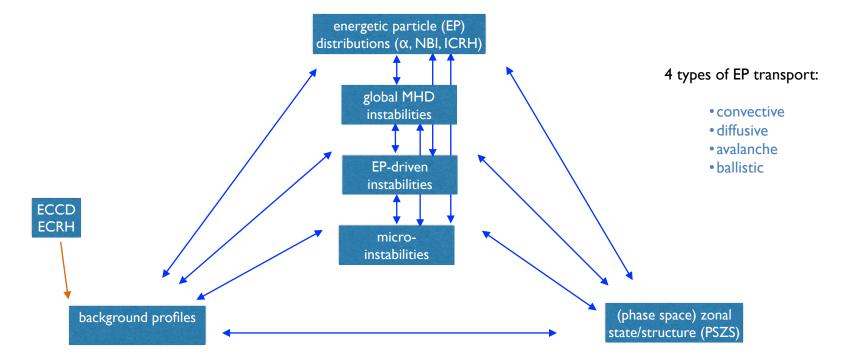
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and A. Bottino, M. Schneider, S.D. Pinches, O. Hoenen, TSVV10 team, ASDEX Upgrade team



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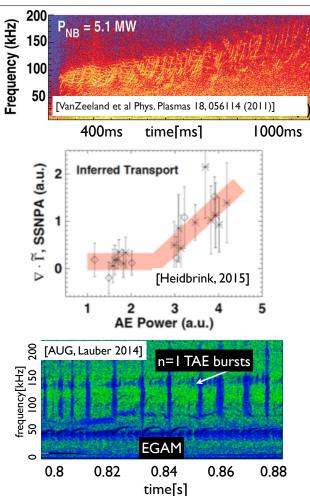
- final goal: predicting the self-organisation of a burning plasma
- challenge: complex interdependence on vastly different spatial and temporal scales

EP transport: experiment



- for multiple overlapping Alfvén eigenmodes (AEs) resonances: stiff EP transport found at DIII-D [Collins, Heidbrink 2015-2018], as predicted by QL theory [Sagedeev&Galeev, Kaufman 1972, ...]; high q, large orbits, dominated by losses rather than redistribution
- in JET re-deposition of EPs (ICRH) was observed: core-localised TAEs redistribute EPs, redistributed EPs drive edge-TAE [Nabais et al, PPCF 2019]
- in ITER, both core and edge TAEs are weakly damped and can be driven non-linearly [Pinches, Lauber, Schneller 2014/2015, T Hayward 2019, ORB5]
- mode chirping and avalanches-type events found in many experiments [Kusama, Shinohara, JT-60U 1999+]
- bursting, non-linear mode-mode couplings and EP transport (FIDA measured in ASDEX Upgrade EP super-shots [Lauber 2014+], .i.e. further development of AUG NLED benchmarks case [Vlad 2020-2023, Vannini 2019, Rettino 2021-23]

for a comprehensive review please refer to dedicated review articles, e.g. [NF ITPA special issue 2006, update 2023/24, Heidbrink 2008, Breizman& Sharapov 2011, Lauber 2013, Chen&Zonca RMP 2015, Gorelenkov&PinchesToi 2014,Todo 2019,...]



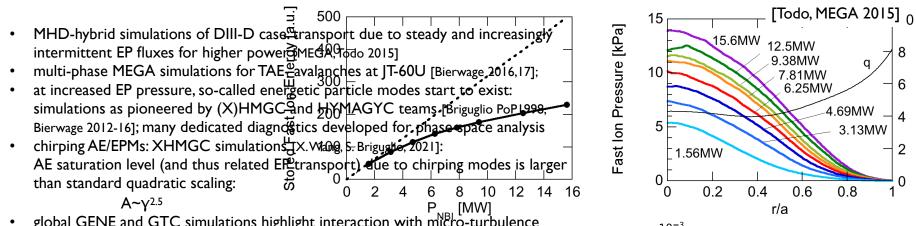
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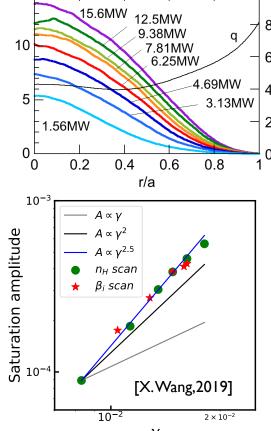
EP transport: modelling



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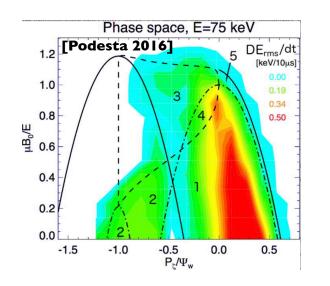


- global GENE and GTC simulations highlight interaction with micro-turbulence [Citrin, diSiena 2019-2023, Brochard 2021-23]
- global ORB5 simulations with increasing complexity start to capture experimentally relevant regimes [A. Biancalani, T Hayward-Schneider, A. Bottino, F.Vannini, B. Rettino 2013-2023] and compare in with MHD-hybrid results [Vlad 2020-23]
- difficult to disentangle various non-linearities in comprehensive codes- verify results?
- transport-time scales?
- vast parameter regime sensitivity scans ?
- how to reduce to reasonably fast models?



- diffusion coefficients for impurity transport by background turbulence, no e.m. EPdriven modes [Angioni 2009, Püschel, etc]
- critical gradient model [R. Waltz, E. Bass, 2014 -2023]: use local AE stability threshold, add upshift of transport threshold using (ExB)_{turb} shearing rate; above threshold set D_{EP} to ad hoc values [e.g. $10m^2/s$] to clamp EP's radial gradient to critical value
- kick model [M. Podesta, 2014-2022]: calculate probability density function of kick in Pz and E for given amplitude
- RBQ model, ID, 2D [N. Gorelenkov 2015-2022]: use resonance broadening QL theory connected to NOVA-K to evolve mode amplitude consistently with evolution of FEP
- gyrofluid model [D Spong, 2019-2022], TAEFL code: fluid closures simplify problem, runs on longer time scales
- GENE-Tango model [A. di Siena, 2022-23]: relies on global kinetic GENE runs + power balance
- transport models as derived from general non-linear gyrokinetic theory [Chen, Zonca RMP 2015, Z. Qiu et a 2017-2023] using phase space zonal structure (PSZS) transport theory [M-V. Falessi, F. Zonca, 2017-2023] see talk M. Falessi at this conference

within Eurofusion Enabling research project ATEP: based on general theoretical framework, develop and implement hierarchy of (reduced) phase space zonal structure (PSZS) transport models



ingredients for reduced energetic particle (EP) transport models:

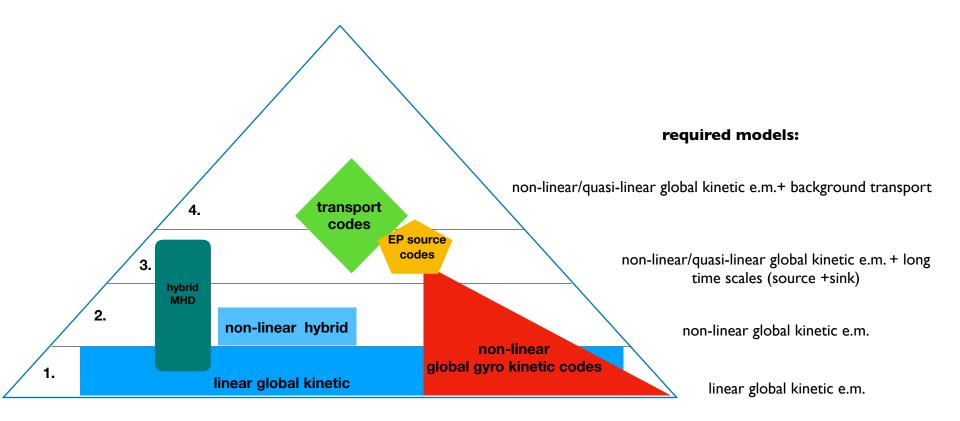
needed for scaling from TCV-AUG-JET, W7X... to JT-60SA-DTT-ITER-DEMO, in particular burning plasmas



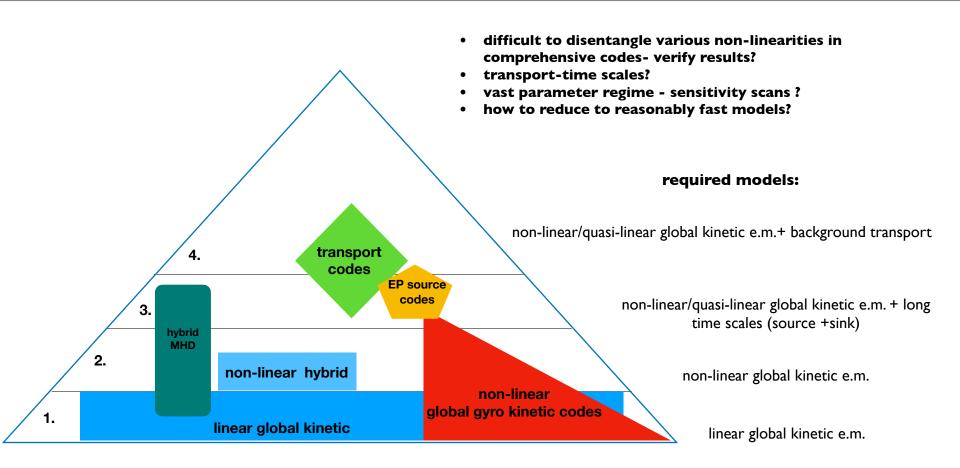
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required models: 4. self-organisation - back reaction of non-linear/quasi-linear global kinetic e.m.+ background transport EP transport on profiles and background transport non-linear/quasi-linear global kinetic e.m. + long time scales (source +sink) 3. EP transport and losses 2. non-linear mode evolution, non-linear global kinetic e.m. saturation mechanisms linear global kinetic e.m. I. mode stability EFTC meeting, Padova, 4.10.2023



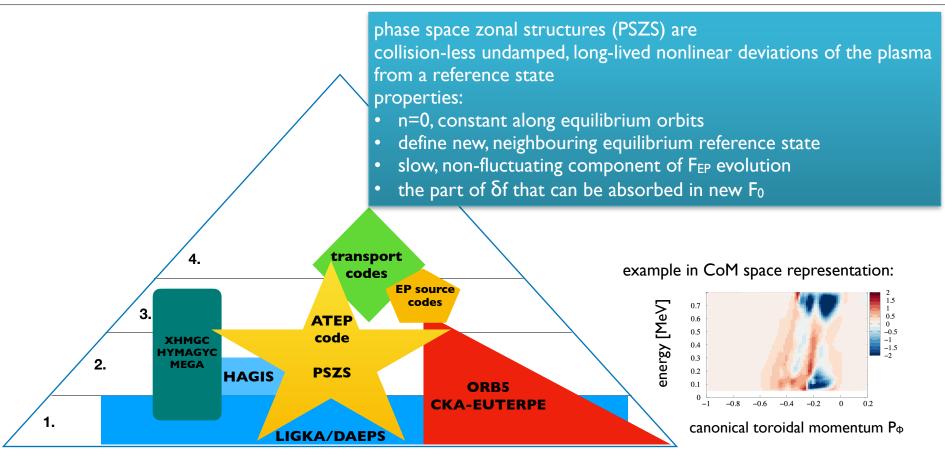






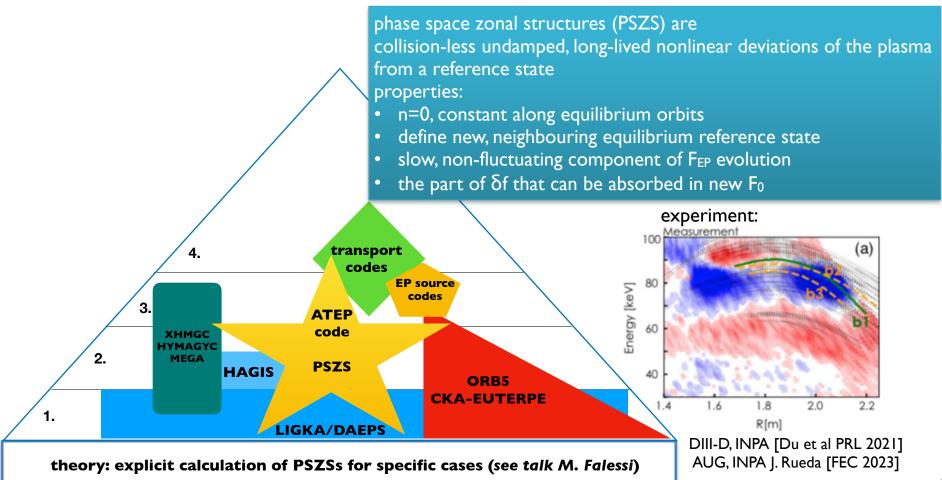
modelling hierarchy for plasmas with significant energetic particle pressure





modelling hierarchy for plasmas with significant energetic particle pressure



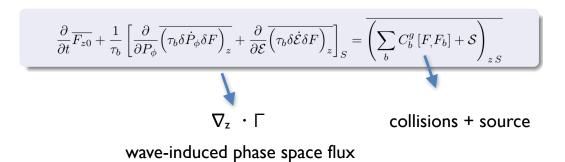




- PSZS theory and overall implementation strategy
- general distribution functions in constants of motion space (CoM)
- linear mode spectrum: the Energetic Particle Stability Workflow (EP-WF)
- phase space transport coefficients
- evolve transport equation in kick model and quasi-linear (QL) limit
- back mapping to real space and non-linear equilibria
- verification and validation common effort of ENR ATEP team

PSZS transport theory and its connection to kick and **QL** limits

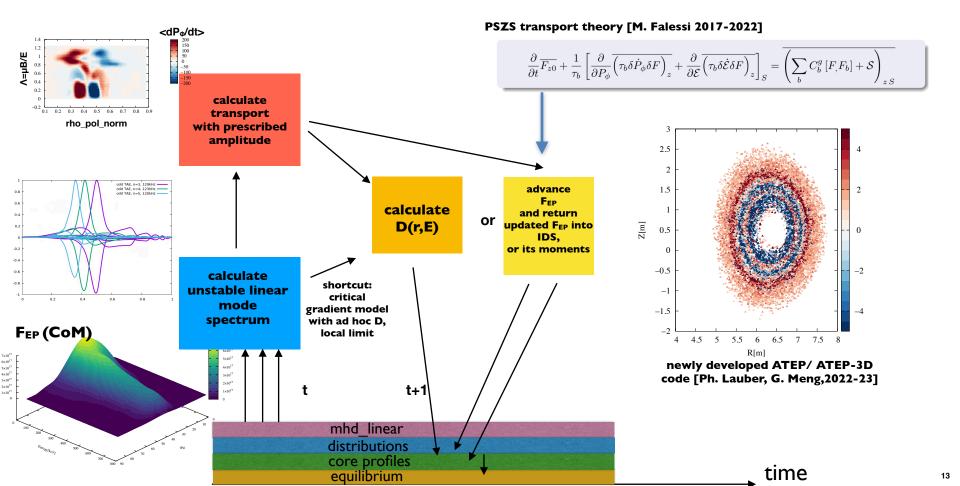




[M-V. Falessi, F. Zonca, 2017-2023] continuity equation in phase space; valid for single or multiple modes in general valid for all regimes; interactions with background fluctuations can be consistently kept

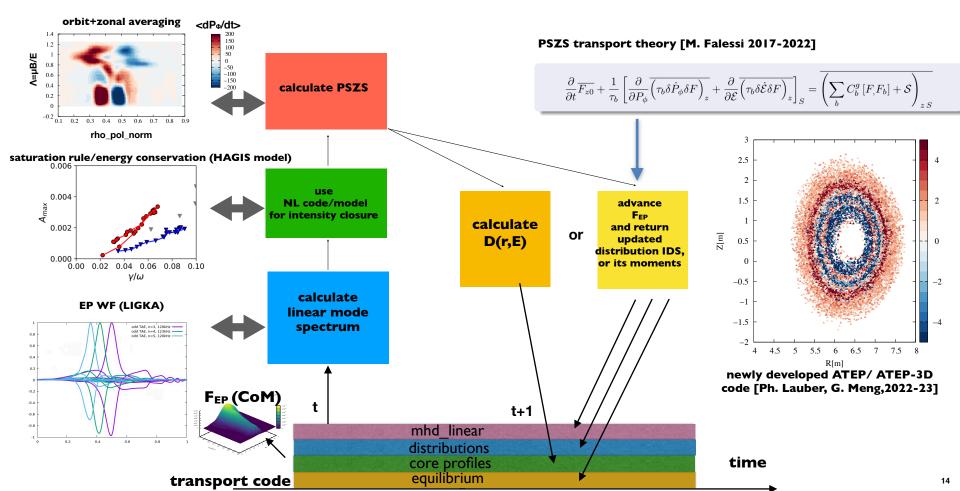
- kick limit: fix perturbations amplitudes for calculating $\langle dP_{\Phi}/dt \rangle$ and evolve continuity equation in CoM space
- in the QL limit, assuming overlapping resonances, flux can be split into convective and diffusive component [L Chen, JGR 104, 1999]
- diffusion coefficients can be evaluated by determining $D_{P\Phi P\Phi} = |dP_{\Phi}/dt|^2 \tau_{ac}$, similar for D_{EE} , and off diagonal terms (if present), resonant and non-resonant contributions can be separated
- in [L Chen, JGR 104, 1999] also the importance of E_{//} is discussed (KAW physics), leading to additional convective flux contributions (linear GK code LIGKA provides this information see below)





implementation: QL limit







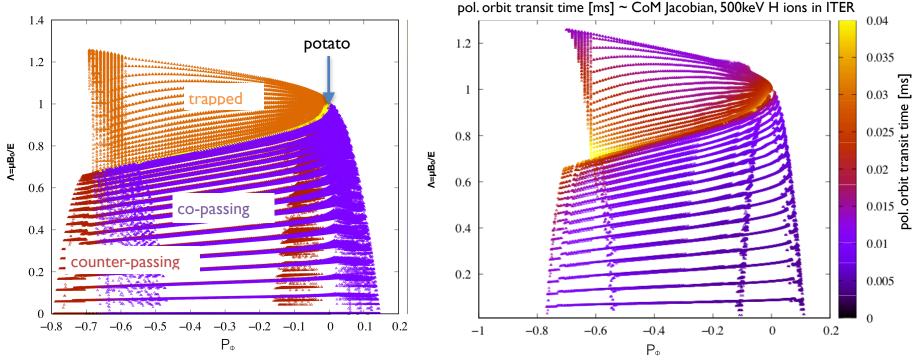
determining FEP in constants of motion space (CoM)

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several recent papers [Bierwage 2022, G. Brochard, FEC 2023, Salewski 2020-21] using a similar procedure:

- establish orbit database to classify particles
- determine CoM Jacobian ($P_{\Phi}, E, \Lambda, \mu B_0/E, \sigma$)
- set up grid in CoM space
- bin markers as given by neoclassical physics codes [NEMO/Spot, ASCOT, RABBIT, etc...], here ITER H-pre-fusion case 100015,1 [M. Schneider, 2018]

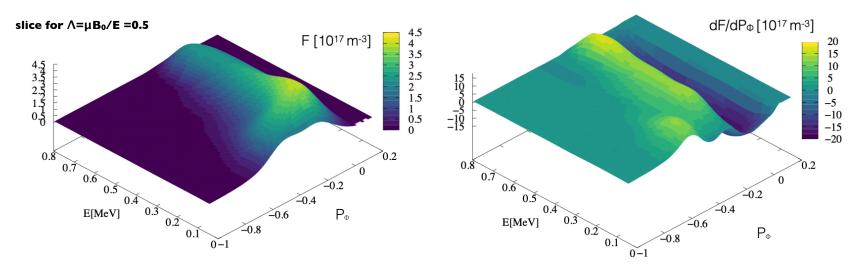


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- use 2D cubic splines in each sub-space to create fine sub-grids, then create 3D spline for FEP
- back-transform in other coordinate systems possible, if needed
- here, all calculations are using IMAS interfaces (equilibrium, transport code, orbit tracer (HAGIS [S.D. Pinches]), ATEP code)



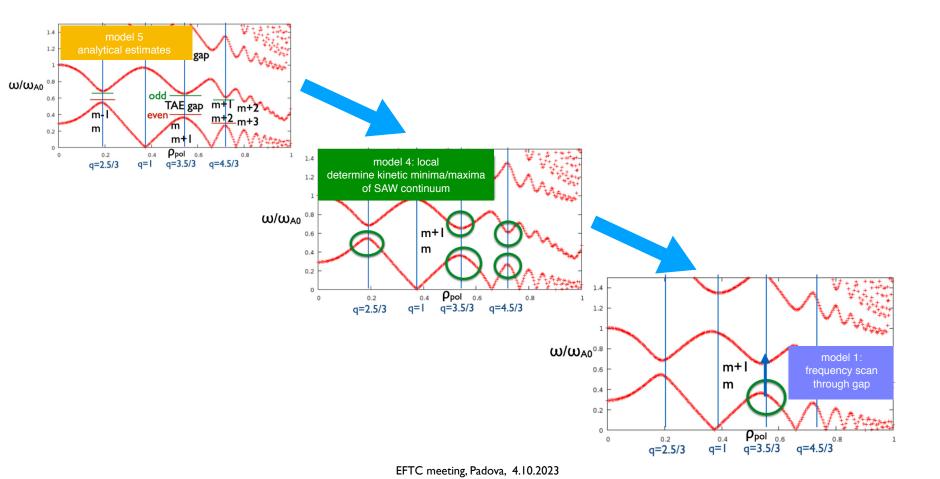


Calculating the mode spectrum

Linear mode spectrum: Energetic particle stability workflow (LIGKA)

LIGKA [Qin 1998, Lauber 2003, JPC 2007, Lauber PLREP 2013, Bierwage&Lauber 2017, Lauber JPCS 2018]

• gyrokinetic moment equation (GKM):
• gyrokinetic moment equation (GKM):
•
$$\frac{\partial}{\partial t} \left[\nabla \cdot \frac{1}{v_{\lambda}^{2}} \nabla_{\perp} \phi \right] + B \cdot \nabla \frac{\nabla \times (\nabla \times (\nabla \psi)_{\|} \psi)}{B} + (b \times \nabla (\frac{\nabla \psi}{i\omega})_{\|} b) \cdot \nabla \frac{\mu o j_{\|}}{B} + (b \times \nabla (\frac{\partial \omega}{2\Omega_{a}})_{\|} b) \cdot \nabla \frac{\mu o j_{\|}}{B} + \sum_{a} \frac{\partial \psi}{\partial \omega} \int \frac{\partial \psi}{\partial \psi} \int \frac{\partial \psi}{\partial \omega} \int \frac{\partial \psi}{\partial \psi} \int \frac{\partial \psi}{\partial \psi}$$



[V.-A. Popa et al 2023 Nucl. Fusion 63]

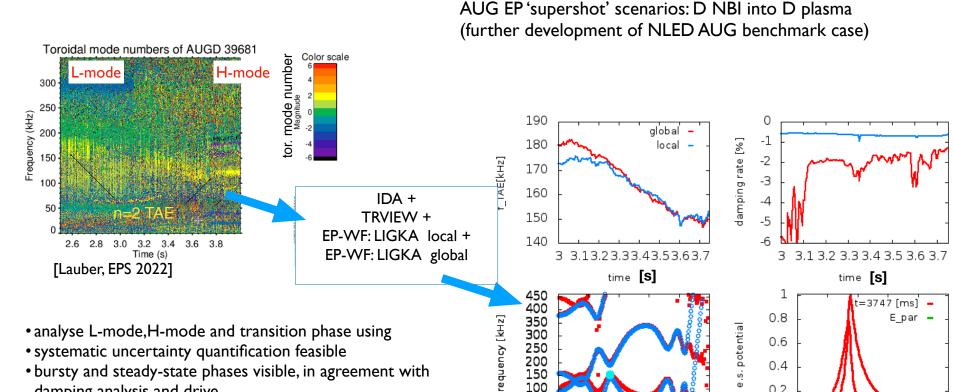
training course & additional material: https://indico.euro-fusion.org/event/2729/

- fully IMAS compatible (python)
- git version control
- module installations available
- gui and non-gui versions
- batch job submission

X -# EP WORKFLOW				X - SPECIES	SETTINGS	• D ×	X - SCENARIO PARAMETER	RS 💶
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run_in	2	Distributions_2	0				n_T	1
machine_out	test_DB	Orbit_Finder	0	Impu	rities		n_Be	1
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Save Configuration as	Load Configuration	SCENARIO Parameters		6	ve Species Configuration	1.4	Save SCENARIO Configu	ration
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🖙 IDS Merge			• • ×					
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machine_in_1	ITER	Equilibrium_copy	~	max_n_tor	10	_		
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		TI D	-	start_pos	1	_		
HDF5_2			1	force_m	false			
Output		ni_Be Ti Be	-	npsi_out	256	_		
machine out	TEST_IDS_MERGE		1	kr_read	0.0d0			
shot out	130012	ni_C	-	q0	0.0d0	_		
run_out	89	Ti_C	-	rad_start	0.0d0			
HDF5_out		ni_Ne Ti Ne		rad_end	1.0d0			
		Ti_Ne		offset_d	0.0d0			
Save IDS_MERGE Configuration				S	ave LIGKA Configuration			

Energetic particle stability workflow: validation at ASDEX Upgrade





damping analysis and drive

• speed up WF using ML methods [V.-A. Popa; in preparation]

100

50

0

0.2

.4

0

.6 0 8

0 radius [r pol] 0.8

0.2

0

0

0.2

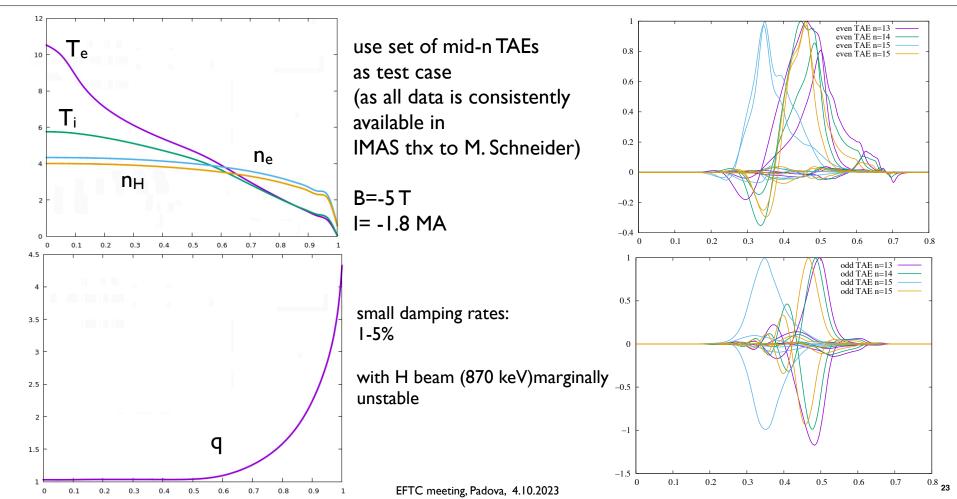
0.6

0.4

radius [r pol]

ITER pre-fusion H scenario 100015,1 [Metis, M. Schneider NF (2021)]

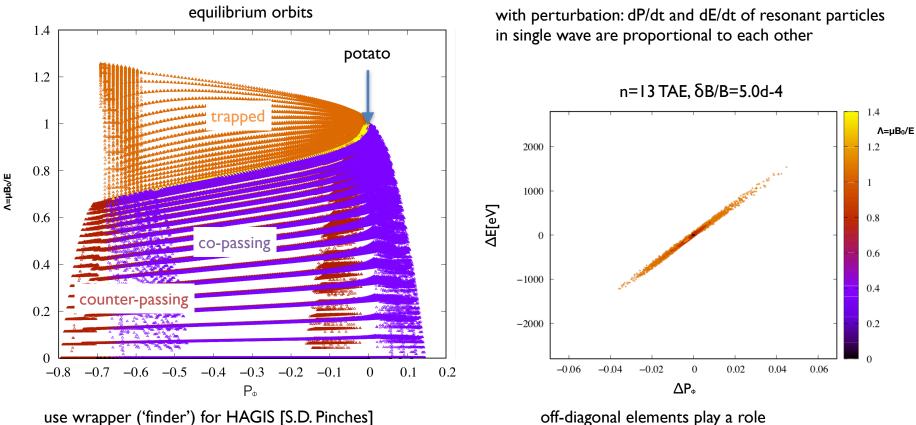






determine phase space transport coefficients





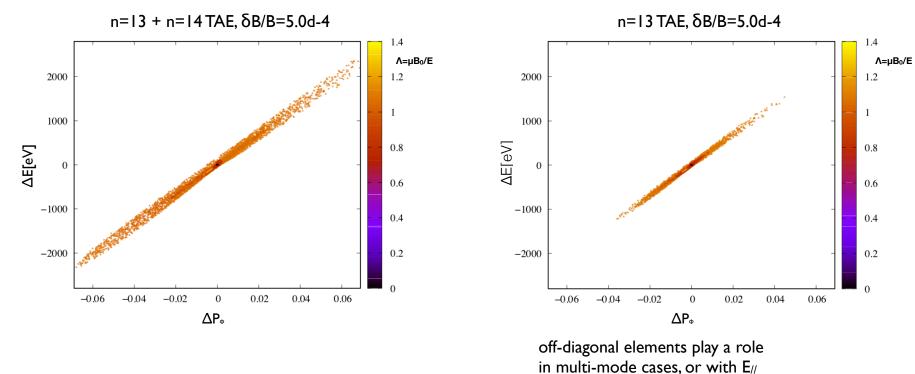
use wrapper ('finder') for HAGIS [S.D. Pinches] to efficiently set up marker space

in multi-mode cases, or with E//

classify particles, calculate orbit properties with and without perturbation(s)



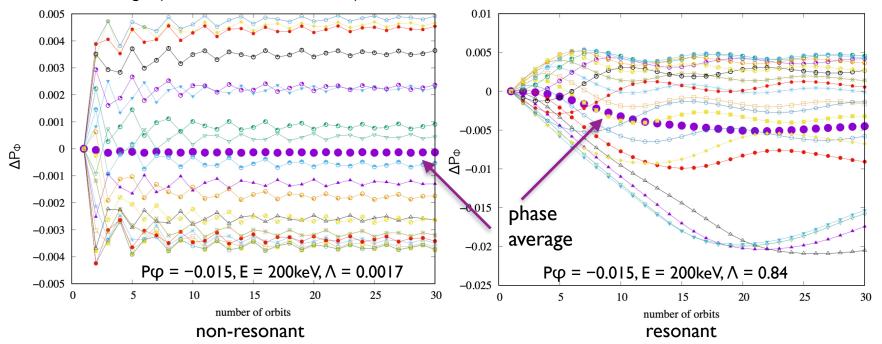
with perturbation: dP/dt and dE/dt of resonant particles in single wave are proportional to each other [Southwood, 1969]



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start particles with different phase shifts with respect to wave: $(2\pi / n, or random)$, follow typical 3-5 orbits to account for higher resonances, then average (n=13TAE; $\delta B/B = 5 \cdot 10-4$)

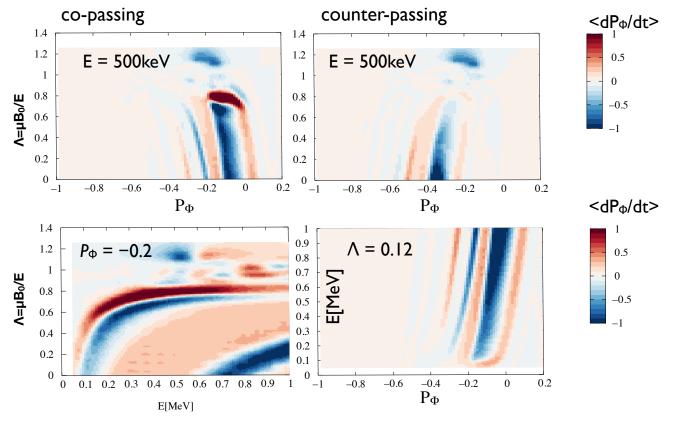


caveat: this procedure is reducing the full dynamics: valid in small-amplitude/QL/limit, transport time scales can be improved, relaxed if needed (ballistic transport cases);

note also close relation to P_{Φ} grid resolution/Courant criterion; accounts for resonance broadening consistently



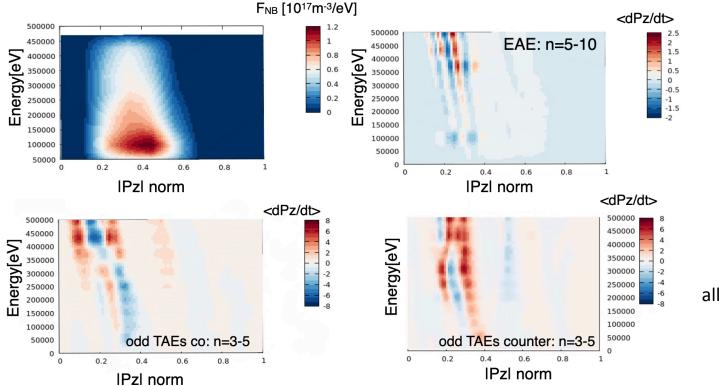
- typically follow
 128x40x40x4 markers
- store in IDS (distributions)
- use multi-level spline interpolation [Lee 1997]
- use cartesian grid in CoM space (96x96x96)



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PSZS for EAEs and odd TAEs





all plots for $\Lambda = \mu B_0 / E = 0.24$

resonances with both positive and negative gradients of F_{EP} possible

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evolve transport equations in kick-model limit

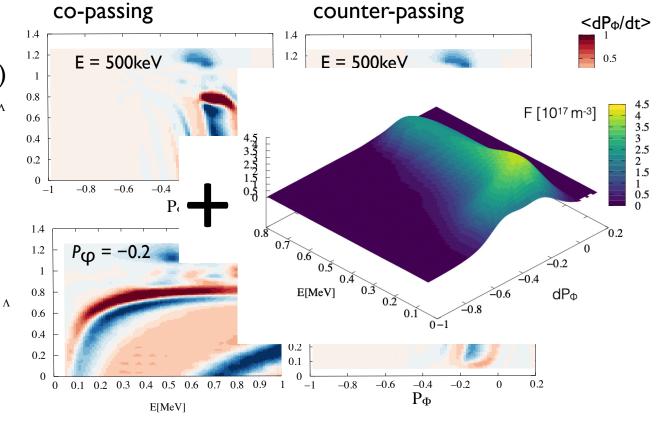


 $\delta B/B = 5 \cdot 10^{-6}$

- typically follow 128x40x40x4 markers
- store in IDS (distributions)

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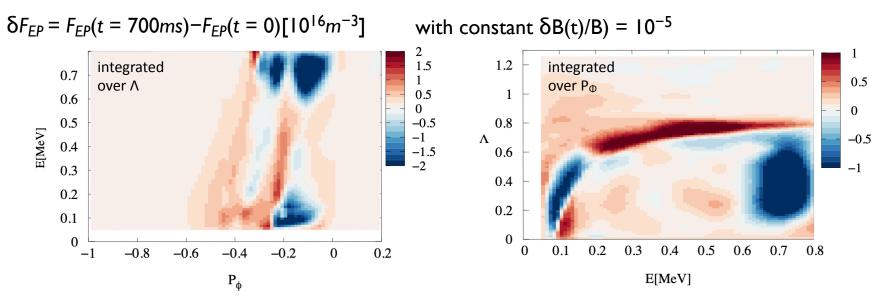
- use multi-level spline interpolation [Lee 1997]
- use cartesian grid in CoM space (96x96x96)





$$\frac{\partial F_z}{\partial t} = -\frac{\partial}{\partial P_{\phi}} \left(\langle \overline{\frac{dP_{\phi}}{dt}} \rangle F_z \right) - \frac{\partial}{\partial E} \left(\langle \overline{\frac{dE}{dt}} \rangle F_z \right) \qquad \mathbf{v}_{P_{\phi},E} = \left(\langle \overline{\frac{dP_{\phi}}{dt}} \rangle, \langle \overline{\frac{dE}{dt}} \rangle \right)$$

advection equation, assuming $\nabla \cdot \mathbf{v}_{P_{\phi},E} = 0$ i.e. incompressible phase space flow is evolved with Lax-Wendroff scheme (explicit, adaptive time step - Courant limit)



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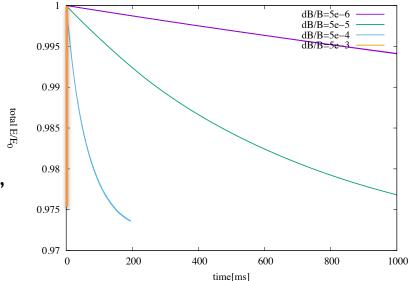
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phase space density is conserved add energy diagnostic:

$$\mathscr{E}(t) = \int dv_{P_{\phi},E,\Lambda} E \cdot F_{EP}(t) / E_0$$

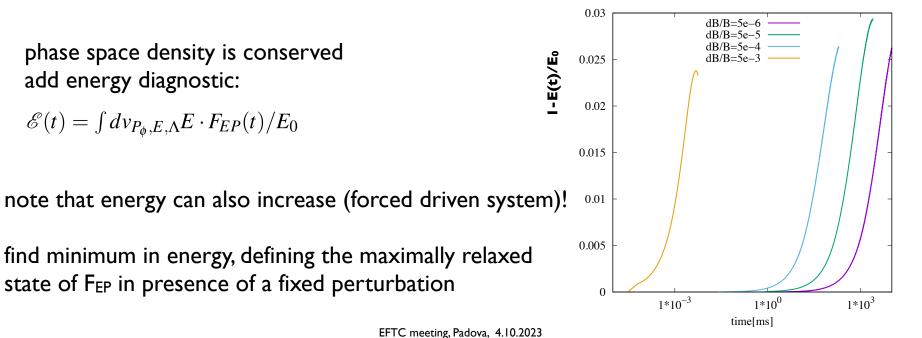
if perturbations are consistently chosen i.e. as unstable eigenfunctions of the equilibrium, energy stored in gradients of F_{EP} is depleted





$$\frac{\partial F_z}{\partial t} = -\frac{\partial}{\partial P_{\phi}} \left(\langle \overline{\frac{dP_{\phi}}{dt}} \rangle F_z \right) - \frac{\partial}{\partial E} \left(\langle \overline{\frac{dE}{dt}} \rangle F_z \right) \qquad \mathbf{v}_{P_{\phi},E} = \left(\langle \overline{\frac{dP_{\phi}}{dt}} \rangle, \langle \overline{\frac{dE}{dt}} \rangle \right)$$

advection equation, assuming $\nabla \cdot \mathbf{v}_{P_{\phi},E} = 0$ i.e. incompressible phase space flow is evolved with Lax-Wendroff scheme (explicit, adaptive time step - Courant limit)





evolve transport equations in quasi-linear limit (QL)

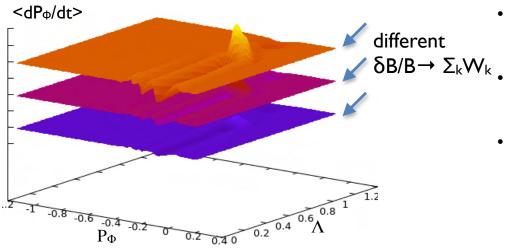


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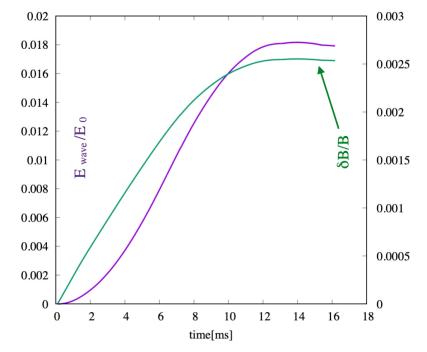
$$\frac{d}{dt}\left(\mathscr{E} + \sum_{k} W_{k}\right) = -2\sum_{k} \gamma_{d,k} W_{k}$$
$$\mathscr{E}(t) = \int dv_{P_{\phi},E,\Lambda} E \cdot F_{EP}(t)$$

amplitude dependent $\langle dP_{\Phi}/dt \rangle$, $\langle dE/dt \rangle$ needed!



- run previously developed WF for calculating PSZS (FINDER/HAGIS) and store in different IDS occurrences
- import into ATEP code (typically 3-5 different amplitudes δ B/B =5 · 10⁻⁶, 5 · 10⁻⁵, 5 · 10⁻⁴, 5 · 10⁻³
- interpolate in CoM space, then construct 4D object
- it includes resonance broadening and transitions from isolated to overlapping modes
- it is NOT yet self-consistent, i.e. ratio of mode amplitudes is fixed (radial envelope equation not solved)
- use E-conservation of PSZS transport equation to determine energy transfer to mode and change mode amplitude(s) accordingly



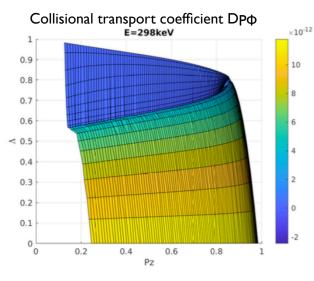


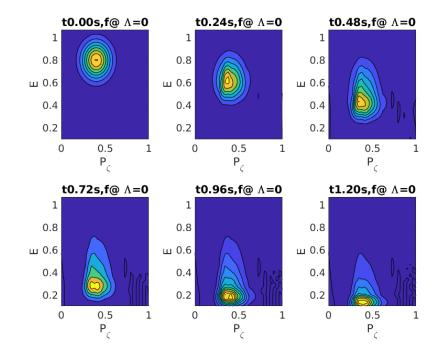
- energy conserving model energy stored in F_{EP} gradients is converted into wave energy: non-linear hybrid model á la HAGIS (non-linear wave particle interaction Lagrangian)
- relative amplitudes of modes remain fixed, as given by linear growth rates ($\gamma^2 \sim A$)
- here, no damping was used yet; mode growth stops after energy of F_{EP} has been exhausted
- for steady state, mode decay has to be balanced by collisions



[Guo Meng, poster at this conference, FEC 2023]

- collision operators are typically given in E, v// space (explicit pitch angle dependence)
- use framework above (IMAS based wrapper for HAGIS) with neoclassical HAGIS version [A. Bergmann, PoP 2001] to obtain orbit-averaged collision coefficients (linearised collision operator)
- use the same CoM grid as for PSZS part
- general 3D solver (implicit solver)
- details: poster G. Meng, at this conference



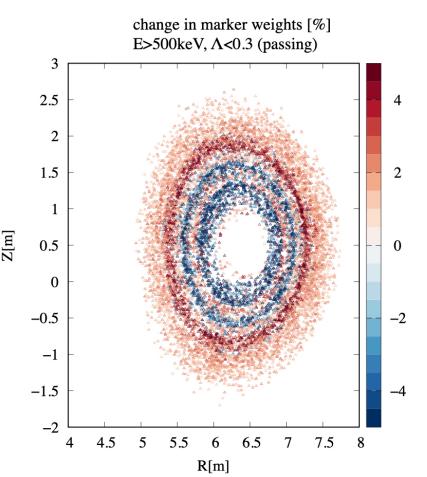


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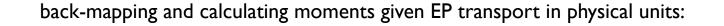


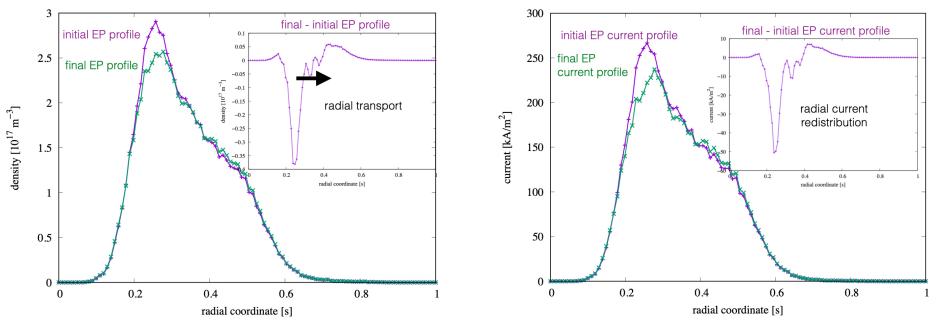
 use map created for setting up orbits quantities (see above) to assign new weights to markers as given by initial input from heating code or SD model

- only 'weights' in CoM are transported, not markers themselves
- transport is by construction 'zonal' taking moments of evolved state allows us to define new non-linear equilibrium:





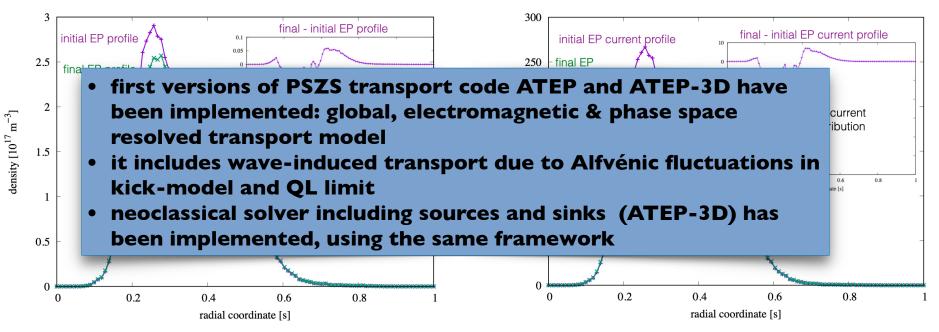




can be passed to transport/equilibrium code to calculate new consistent non-linear equilibrium



back-mapping and calculating moments given EP transport in physical units:



can be passed to transport/equilibrium code to calculate new consistent non-linear equilibrium





verify, validate and evolve models - ENR ATEP team effort



verify, validate and evolve models - ENR ATEP group

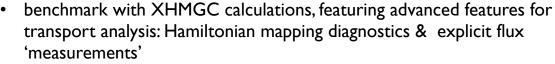


- benchmark with original HAGIS model
- benchmark with DAEPS code calculates fluxes explicitly based on separation of radial and parallel mode structures
- started extension to 3D geometry [A. Zocco, 2023]
- benchmark with ID beam-plasma system [N. Carlevaro, PPCF 2022]:
 - bump on tail model
 - partition phase space in slides of maximal power exchange
 - use LIGKA linear mode information
 - successful comparison with LIGKA-HAGIS model
- tracers dynamics studied with Lagrangian Coherent structures: relevant structures/barriers change during non-linear evolution: from inner to outer radial transport peak (see ITER case above):

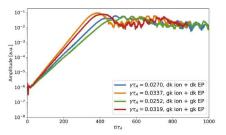
add tracers to system an determine diffusive (T) vs. convective (T^2) scaling: τ=0. s₀≈0.3 _ τ=510 [103] τ=840 df_H/ds τ=1272 S² s₀≈0.6 N. Carlevaro et al, EPS22 700 800 1300 1400 0.4 0.8 0.3 0.6 s 0.020 0.010 0.005 As time increases the more robust 0.015 0.015 barriers move radial outwards (avalanche mode excitation) 0.005 0.35 0.40 0.45 0.50 0.55 0.60 0.65 0.70 0.50 0.55 0.60 0.65 0.70 0.35 0.40 0.45 0.50 0.55 0.60 0.65 0.70 0.015 43

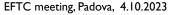
verify, validate and evolve models - ENR ATEP group

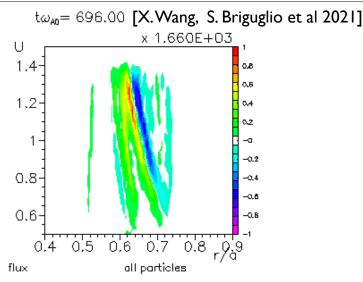


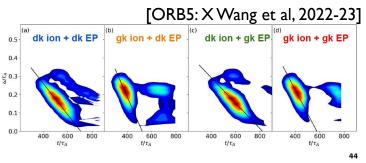


- implemented also in HYMAGYC [G.Vlad, V. Fusco]
- benchmark with STRUPHY code: MHD-kinetic hybrid code based on new stringent mathematical formulation: structure preserving geometric finite elements + PIC ⇒ improved non-linear stability [F Holderried, S Possanner 2020-2023]
- compare with ORB5 PSZS diagnostics [A. Bottino Varenna 2022] (see talk M. Falessi) compare to various ORB5 results; e.g. use scaling for chirping modes ORB5 runs are available also in presence of turbulence
- analyse and plan new experiments based on AUG EP 'Supershots' INPA measurements of phase space transport !
 []. R. Rueda, FEC 2023]





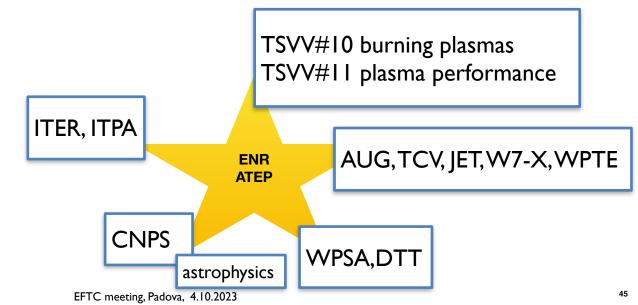






started enable new routes to EP transport analysis and prediction via:

- new theoretical framework
- new common concept of connecting non-linear code results to reduced models (PSZS)
- new common EP transport code developments
- newly implemented analysis methods
- new IMAS based infrastructure



established and growing connections to other groups and experiments