MAX-PLANCK-INSTITUT
FÜR PLASMAPHYSIK

On the implementation of advanced energetic particle transport models

Ph. Lauber, V.-A. Popa, T. Hayward-Schneider, M.-V. Falessi

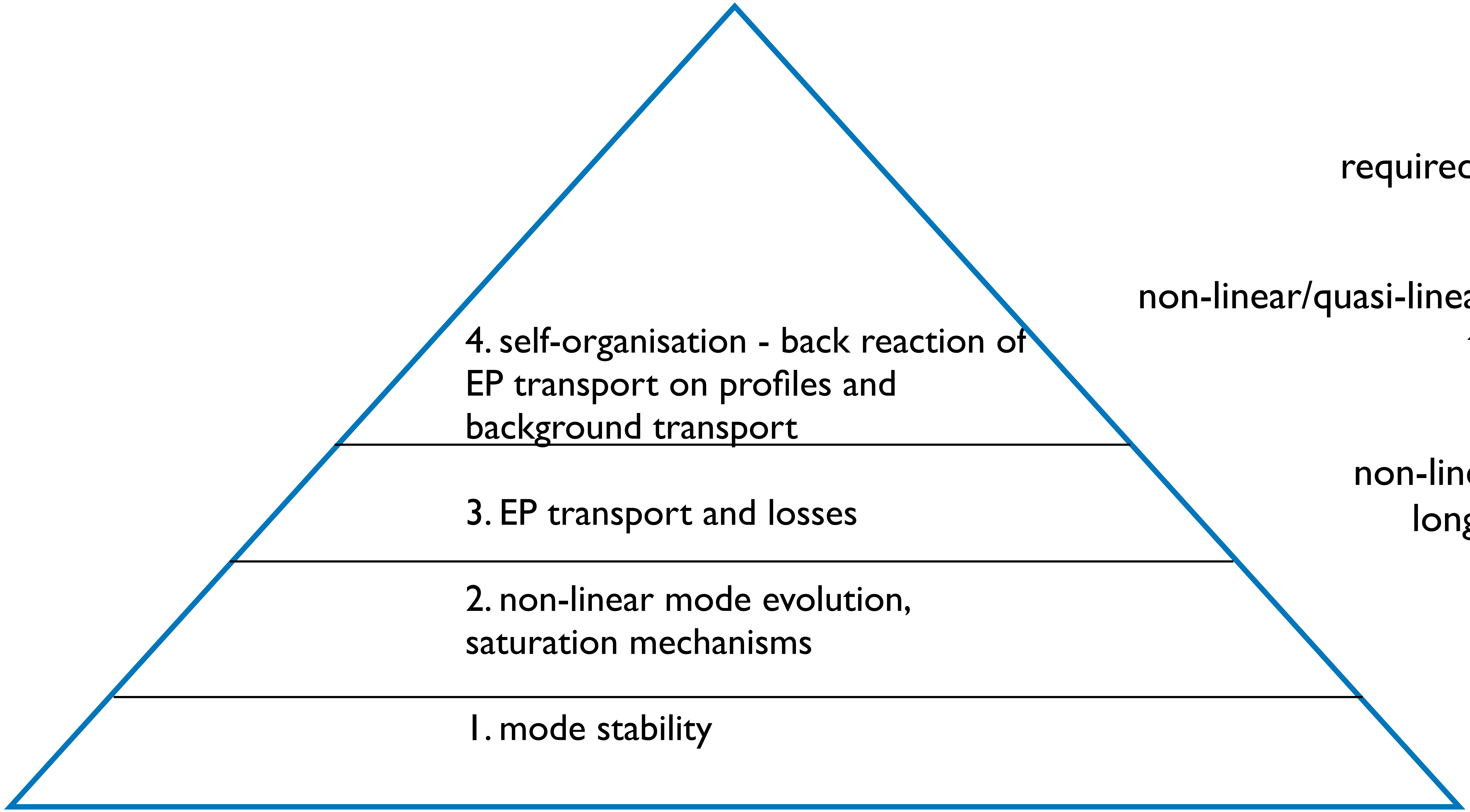
acknowledgements: ATEP ENR team,
F. Zonca, S.D. Pinches, M. Schneider, O. Hoenen

ENR ATEP: https://wiki.euro-fusion.org/wiki/Project_No10

https://indico.euro-fusion.org/category/309/

modelling hierarchy for plasmas with significant energetic particle pressure

needed for scaling from TCV-AUG-JET,… to JT-60SA-DTT-ITER-DEMO:



required model:

non-linear/quasi-linear global kinetic + background transport

non-linear/quasi-linear global kinetic + long time scales (source +sink)

non-linear global kinetic

linear global kinetic

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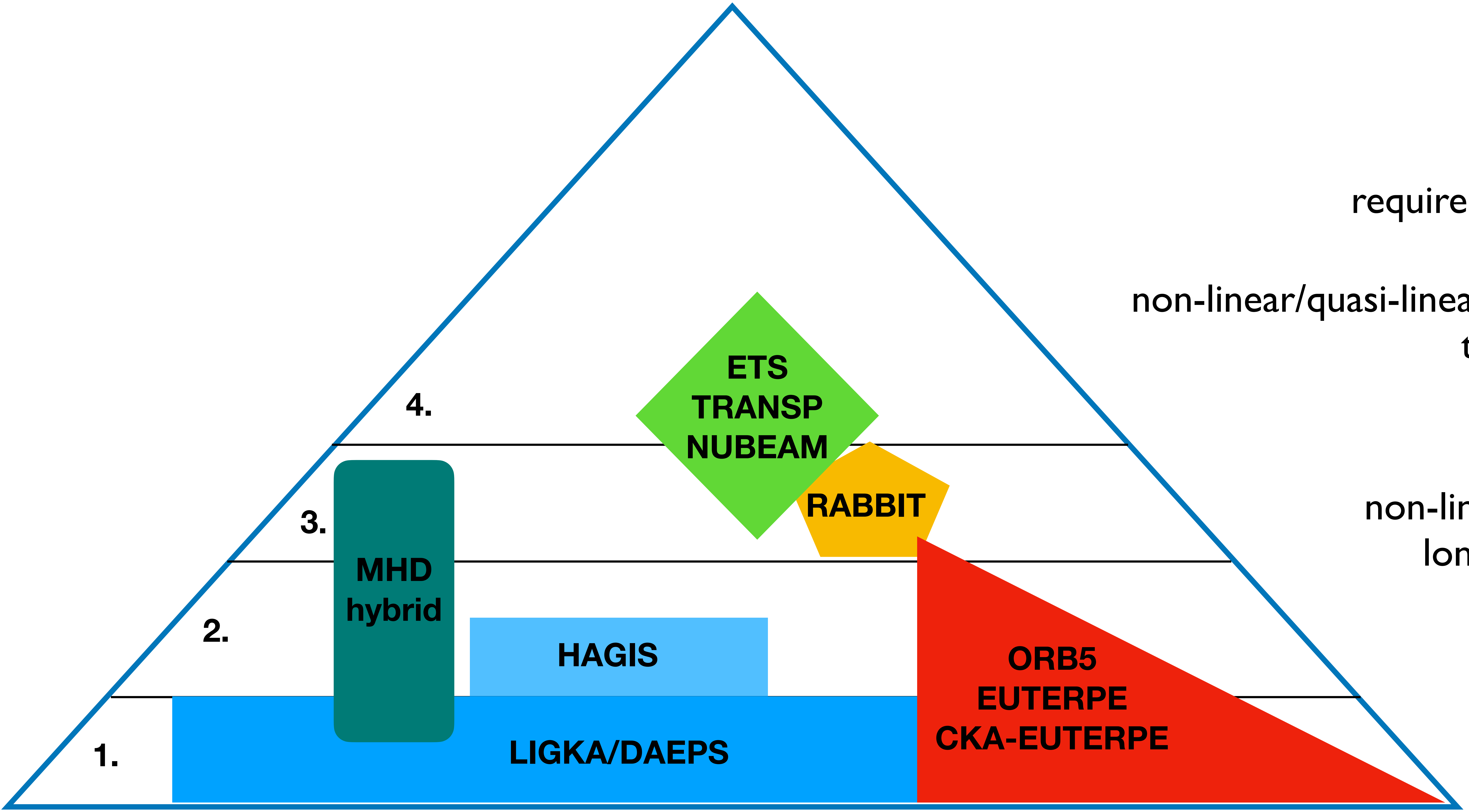

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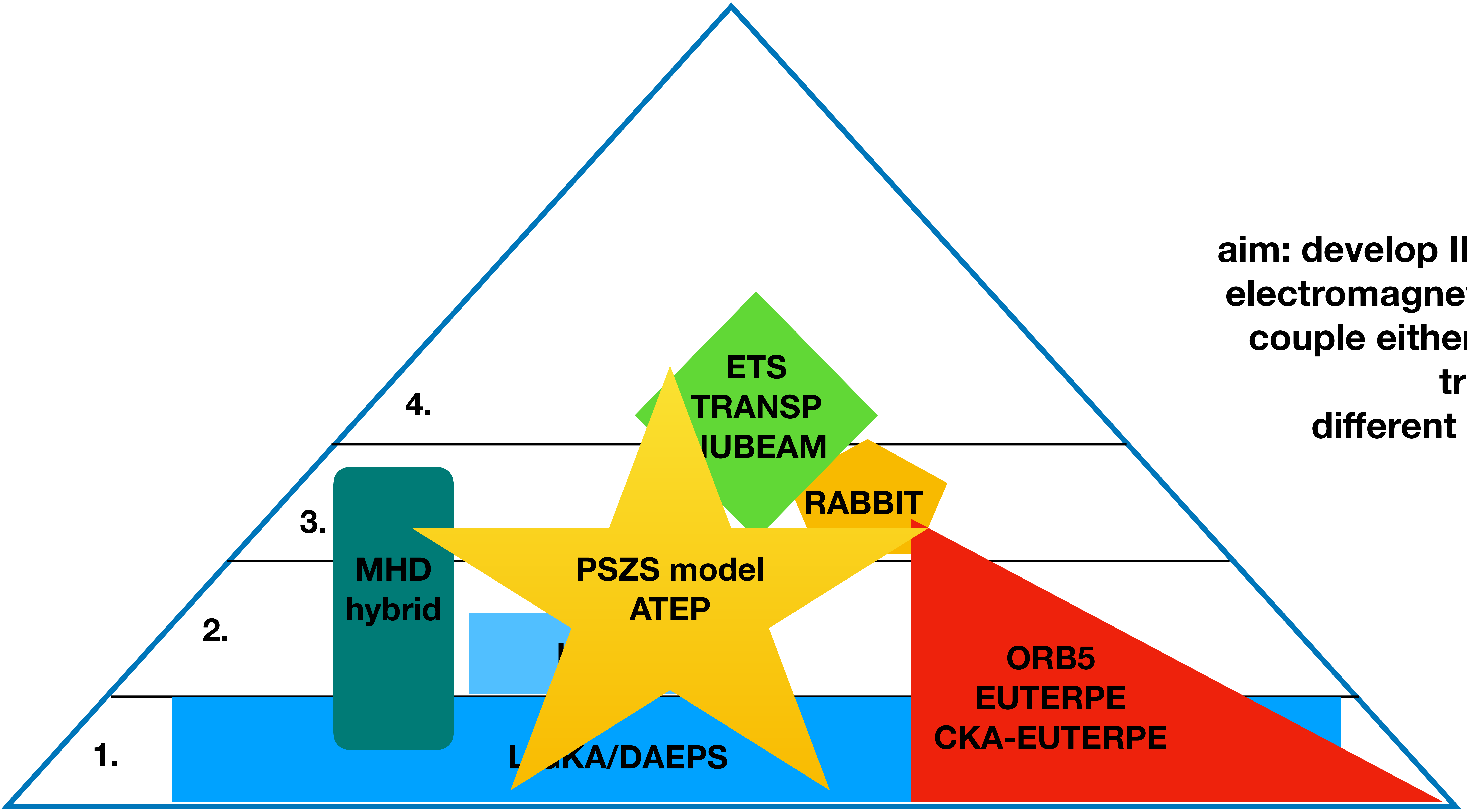


aim: develop IMAS based tool to calculate electromagnetic, global EP transport and couple either via F_{EP} or its moments to transport codes; different models of fidelity/cost

formulation of transport processes in available transport codes:

e.g. ETS:

[D. Coster et al IEEE TRANSACTIONS ON PLASMA SCIENCE, VOL. 38, 2010]

$$\rightarrow \frac{\partial n}{\partial t} = -\nabla \cdot \vec{\Gamma} + S$$

$$\vec{\Gamma} = -D\nabla n + n\vec{v}$$

$$\sigma_{\parallel}\left(\frac{\partial}{\partial t} - \frac{\rho \dot{B}_0}{2B_0} \cdot \frac{\partial}{\partial \rho}\right)\Psi = \frac{F^2}{\mu_0 B_0 \rho}\frac{\partial}{\partial \rho}\left[\frac{V'}{4\pi^2}\left\langle\left|\frac{\nabla\rho}{R}\right|^2\right\rangle\frac{1}{F}\frac{\partial \Psi}{\partial \rho}\right] - \frac{V'}{2\pi\rho}(j_{\mathrm{ni,exp}} + j_{\mathrm{ni,imp}} \cdot \Psi) \qquad (1)$$

a density equation for each ion species

$$\left(\frac{\partial}{\partial t} - \frac{\dot{B}_0}{2B_0} \cdot \frac{\partial}{\partial \rho}\rho\right)(V' n_i) + \frac{\partial}{\partial \rho}\Gamma_i = V'(S_{i,\mathrm{exp}} - S_{i,\mathrm{imp}} \cdot n_i) \qquad (2)$$

a temperature equation for each ion species

$$\frac{3}{2}\left(\frac{\partial}{\partial t} - \frac{\dot{B}_0}{2B_0} \cdot \frac{\partial}{\partial \rho}\rho\right)\left(n_i T_i V'^{\frac{5}{3}}\right) + V'^{\frac{2}{3}}\frac{\partial}{\partial \rho}(q_i + T_i\gamma_i) = V'^{\frac{5}{3}}[Q_{i,\mathrm{exp}} - Q_{i,\mathrm{imp}} \cdot T_i + Q_{\mathrm{ei}} + Q_{\mathrm{zi}} + Q_{\gamma i}] \qquad (3)$$

a temperature equation for the electrons

$$\frac{3}{2}\left(\frac{\partial}{\partial t} - \frac{\dot{B}_0}{2B_0} \cdot \frac{\partial}{\partial \rho}\rho\right)\left(n_e T_e V'^{\frac{5}{3}}\right) + V'^{\frac{2}{3}}\frac{\partial}{\partial \rho}(q_e + T_e\gamma_e) = V'^{\frac{5}{3}}[Q_{e,\mathrm{exp}} - Q_{e,\mathrm{imp}} \cdot T_e + Q_{\mathrm{ie}} - Q_{\gamma i}] \qquad (4)$$

some existing transport models for EPs

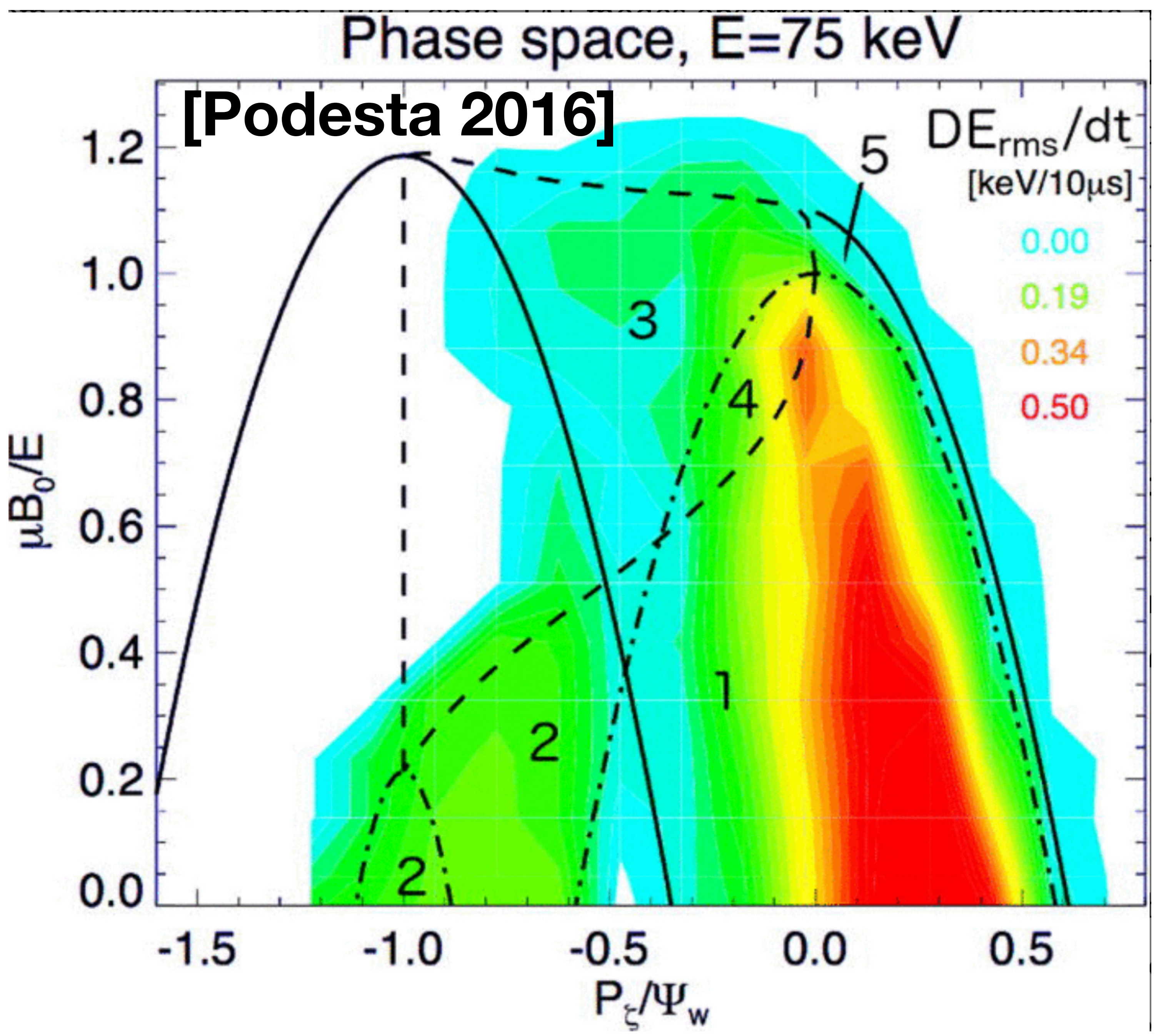
- diffusion coefficients for impurity transport by background turbulence, no e.m. EP-driven modes [Angioni, Püschel, etc]

- critical gradient model [R. Waltz, E. Bass]: use local AE stability threshold, add upshift of transport threshold using $(ExB)_{turb}$ shearing rate; above threshold set DEP to ad hoc values [e.g. $10 m^2/s$] 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, 1D, 2D [N. Gorelenkov 2015-2022]: use resonance broadening QL theory connected to NOVA-K to evolve mode amplitude consistently with evolution of F_{EP}

- PSZS model [M-V. Falessi, 2017-2021] - consistently embedded in general NL GK theory [see e.g. talk F. Zonca PPPL EP Seminar May 2022] gives clear guidance on validity and limitations of reduced models by monitoring simplification conditions



kick model/ quasi-linear diffusion model

typical quasi-linear scheme:

$$\gamma_n = 2\pi^2 \frac{e^2}{m} \frac{v_n}{|k_n|} \frac{\partial f(v_n)}{\partial v}$$

$$\frac{\partial}{\partial t} W_n = 2\gamma_n W_n$$

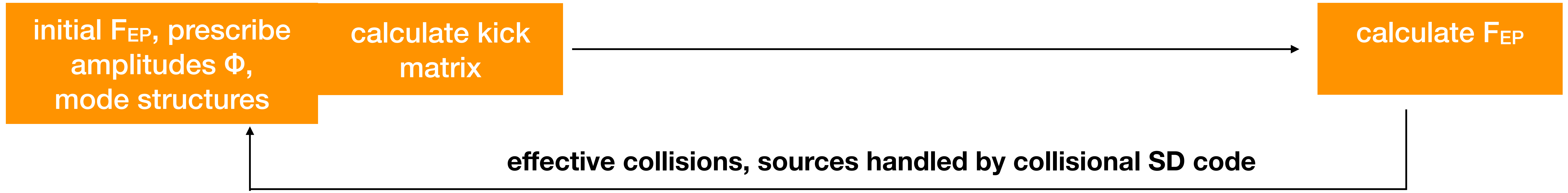
$$W_n = \frac{|k_n \phi_{n0}|^2}{2\pi\, v_n}$$

$$D(v) = \frac{2\pi e^2}{m^2} \sum_n |k_n \phi_{n0}|^2 \, \delta(\Omega_n)$$

+self consistent resonance broadening

$$\frac{\partial f}{\partial t} = \widehat{Q} f \equiv \frac{\partial}{\partial v}\left(D(v) \frac{\partial f}{\partial v} \right)$$

kick model scheme:



phase space zonal structure transport theory

[M.-V. Falessi, 2017-2021]
[L. Chen JGR, 1999]

start from NL GK equation,
and derive evolution equation of toroidally symmetric component due to fluctuations and sources/collisions:

$$\frac{\partial}{\partial t}\overline{F_{z0}} + \frac{1}{\tau_b}\left[\frac{\partial}{\partial P_\phi}\overline{\left(\tau_b \delta \dot{P}_\phi \delta F\right)}_z + \frac{\partial}{\partial \mathcal{E}}\overline{\left(\tau_b \delta \dot{\mathcal{E}} \delta F\right)}_z\right]_S = \overline{\left(\sum_b C_b^g\left[F, F_b\right] + \mathcal{S}\right)}_{zS}$$

splitting micro and meso/macro scales - describes evolution of non-linear equilibrium including long-lived n=0 structures from perturbations

use connection to QL GK equations to reconcile with QL transport theory, e.g. in [L. Chen JGR, 1999]

$$\frac{\partial}{\partial t}(B_\parallel^* F_o) + \bar{\nabla}\cdot(B_\parallel^* \dot{\mathbf{X}}_o F_o) + \frac{\partial}{\partial w}(B_\parallel^* w_o F_o) + \bar{\nabla}\cdot(B_\parallel^* \overline{\delta\dot{\mathbf{X}}\delta G_{\rm res}})$$
$$+ \frac{\partial}{\partial w}(B_\parallel^* \overline{\delta\dot{w}\delta G_{\rm res}}) = 0 \qquad (12)$$

mapping from Pz,E,μ space to real space:

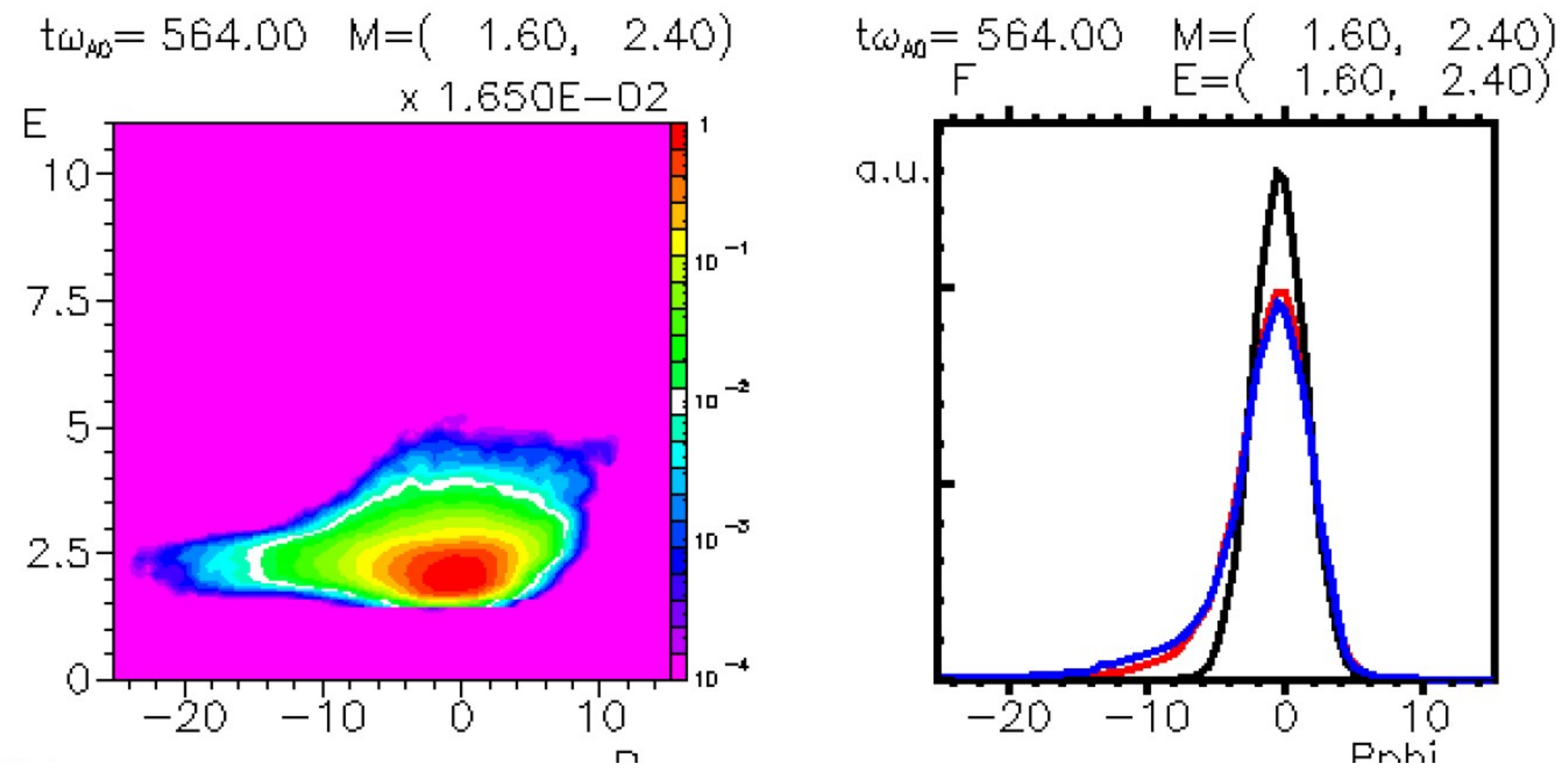
$$D_{\psi\psi} = \overline{\delta\dot{\psi}\delta\dot{\psi}}\tau_{ac} = \frac{1}{2}\sum_{\omega,\mathbf{k}_\perp} c^2 m_\beta^2 |\delta\hat{\Phi}|^2 \tau_{ac} \qquad (45)$$

$$D_{\psi\varepsilon} = D_{\varepsilon\psi} = \overline{\delta\dot{\psi}\delta\dot{\varepsilon}}\tau_{ac} = \frac{1}{2}\sum_{\omega,\mathbf{k}_\perp} c m_\beta \frac{\omega e}{m}|\delta\hat{\Phi}|^2 \tau_{ac} \qquad (46)$$

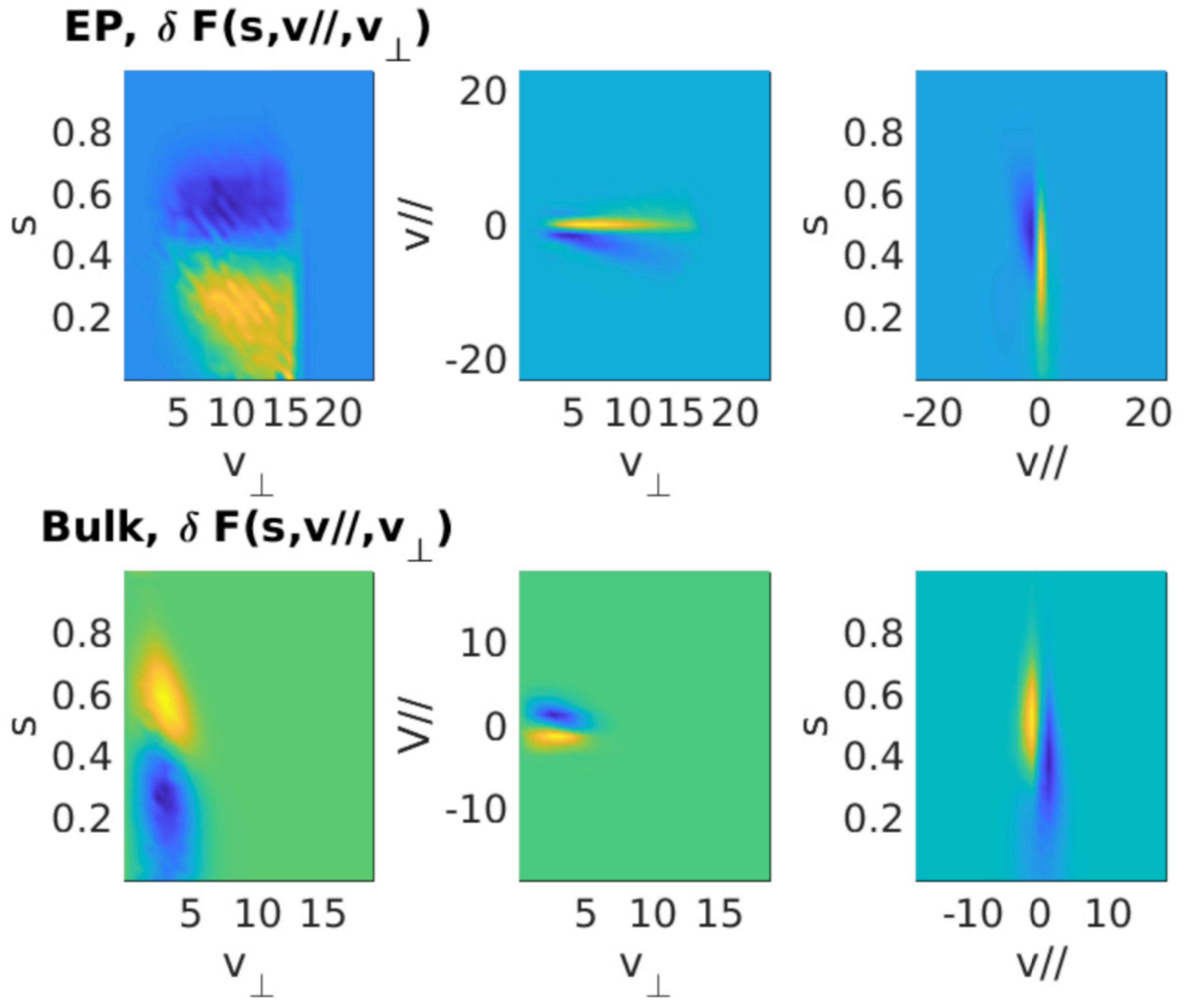
$$D_{\varepsilon\varepsilon} = \overline{\delta\dot{\varepsilon}\delta\dot{\varepsilon}}\tau_{ac} = \frac{1}{2}\sum_{\omega,\mathbf{k}_\perp}\left(\frac{\omega e}{m}\right)^2 |\delta\hat{\Phi}|^2 \tau_{ac} \qquad (47)$$

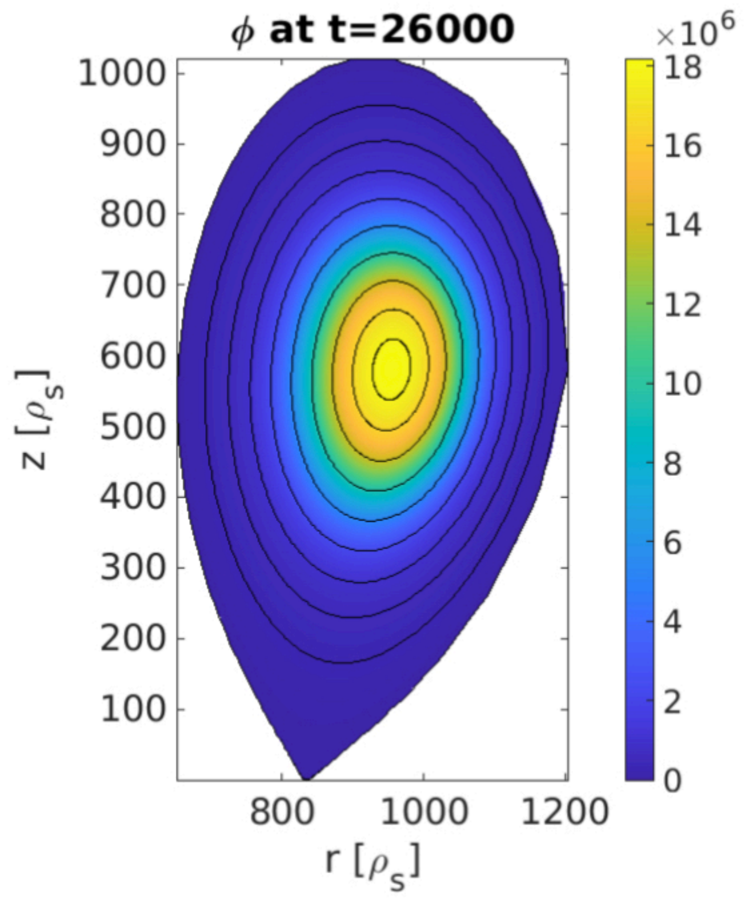
implementation of PSZS in NL MHD-hybrid and GK codes

PSZSs have been extracted from HMGC and HYMAGYC MHD-kinetic hybrid codes
[S. Briguglio, G. Vlad et al 2019-2022]

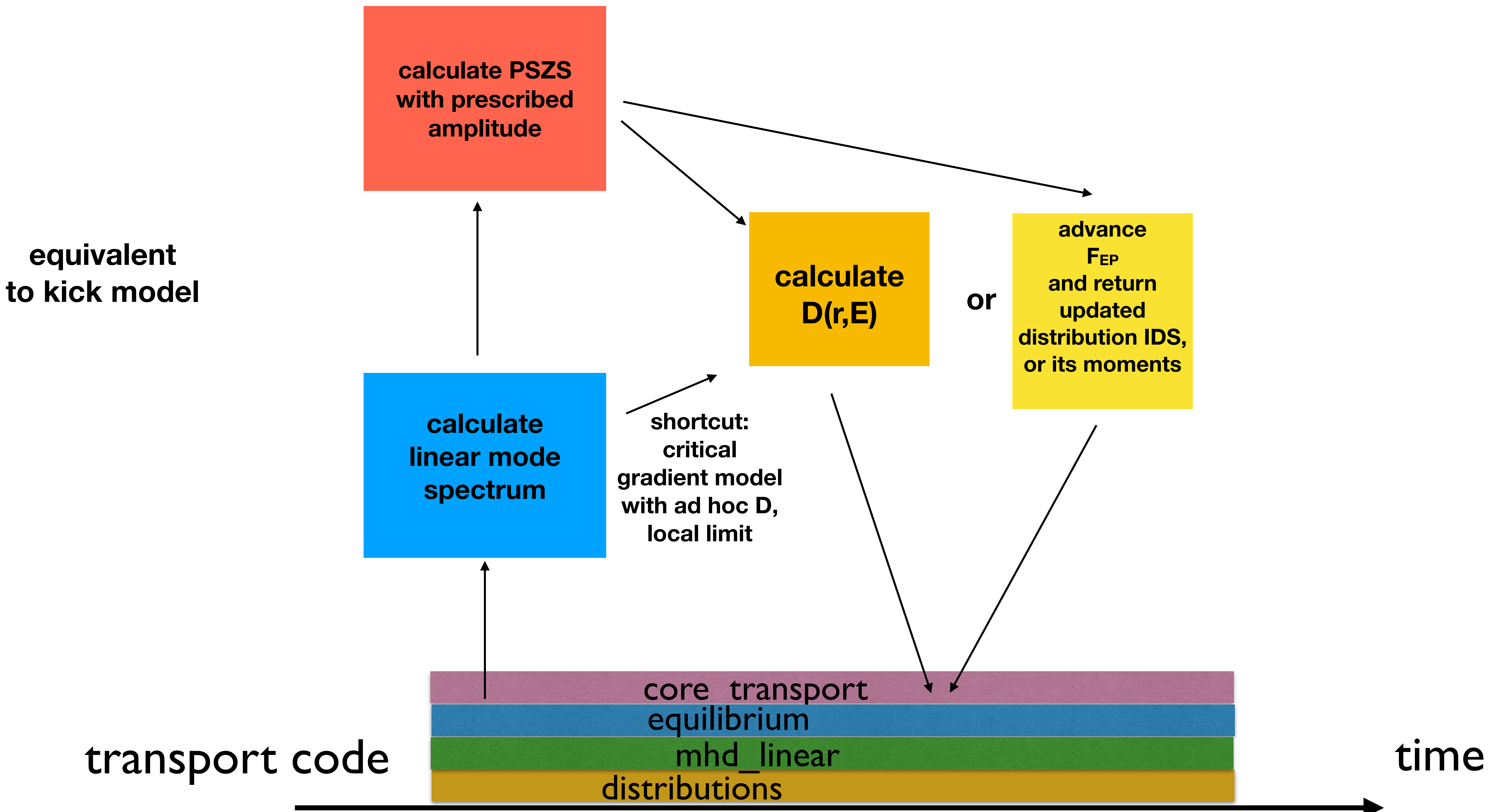


recently also in non-linear GK code ORB5
NLED AUG EPM/TAE [A. Bottino, ATEP seminar, 3/2022]

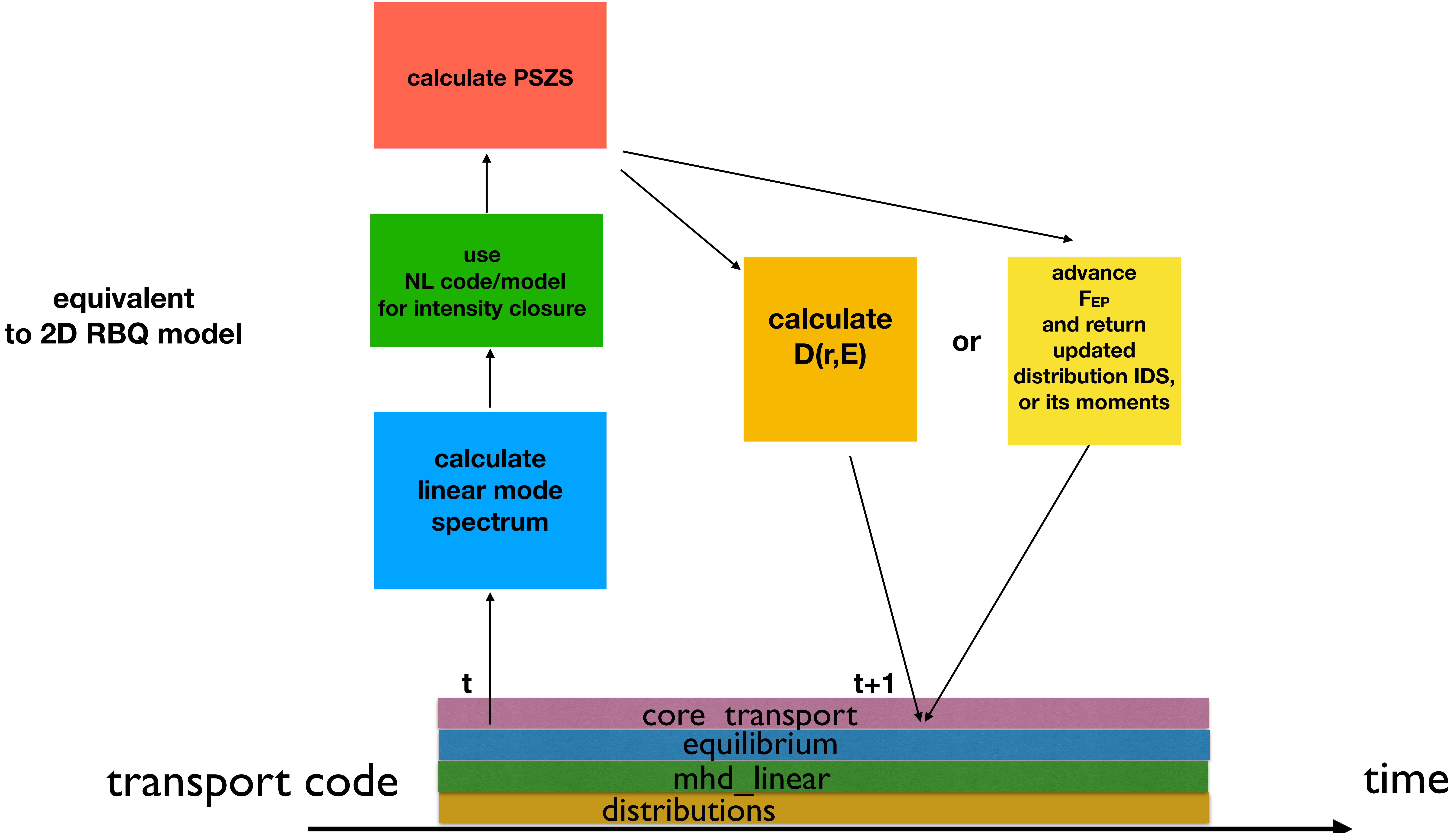




outline: ATEP framework
EP transport workflow schematics

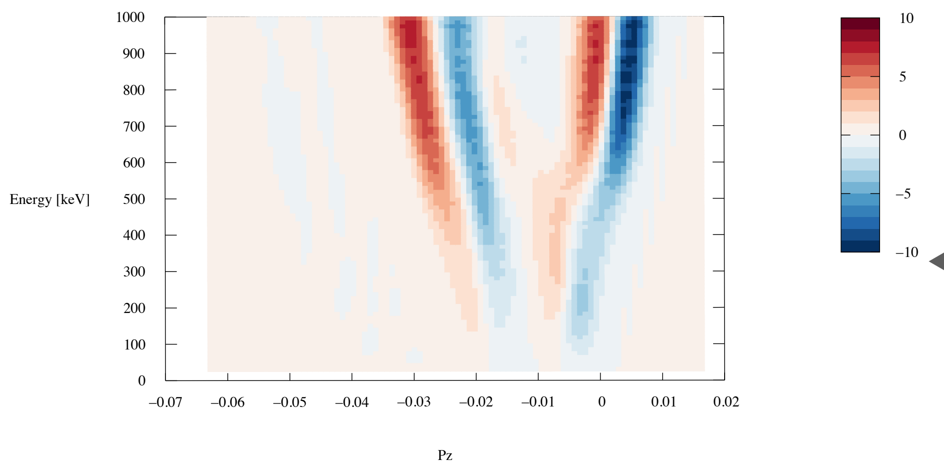


EP transport workflow schematics

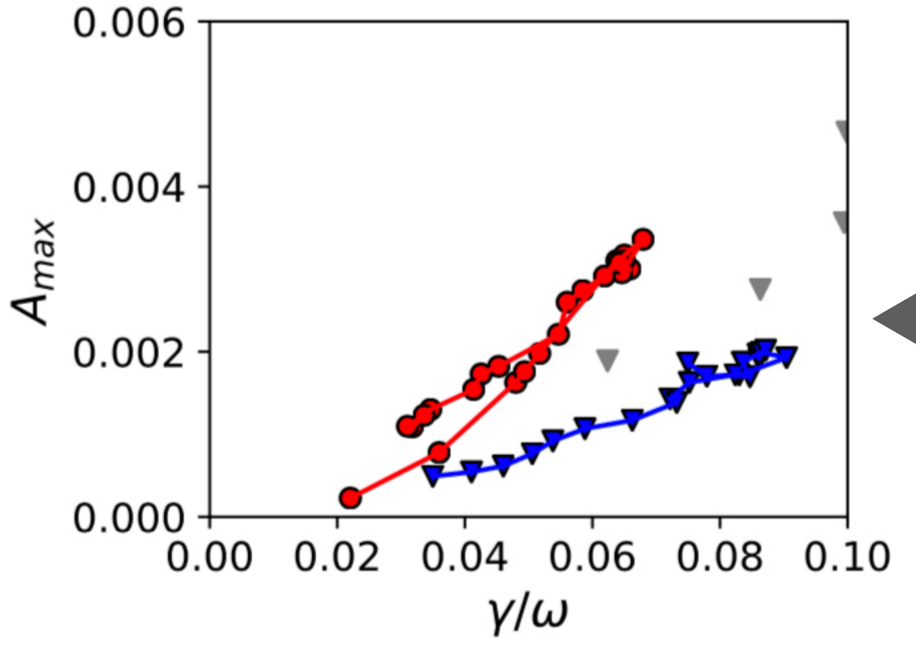


EP transport workflow schematics

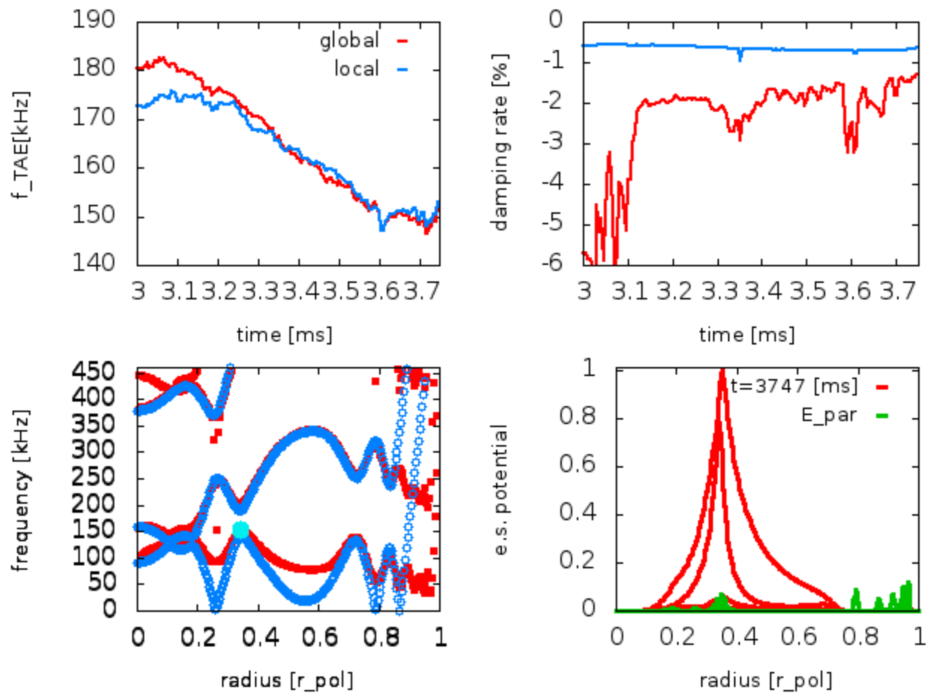
FINDER/HAGIS [Ph. Lauber, 2007,2022]

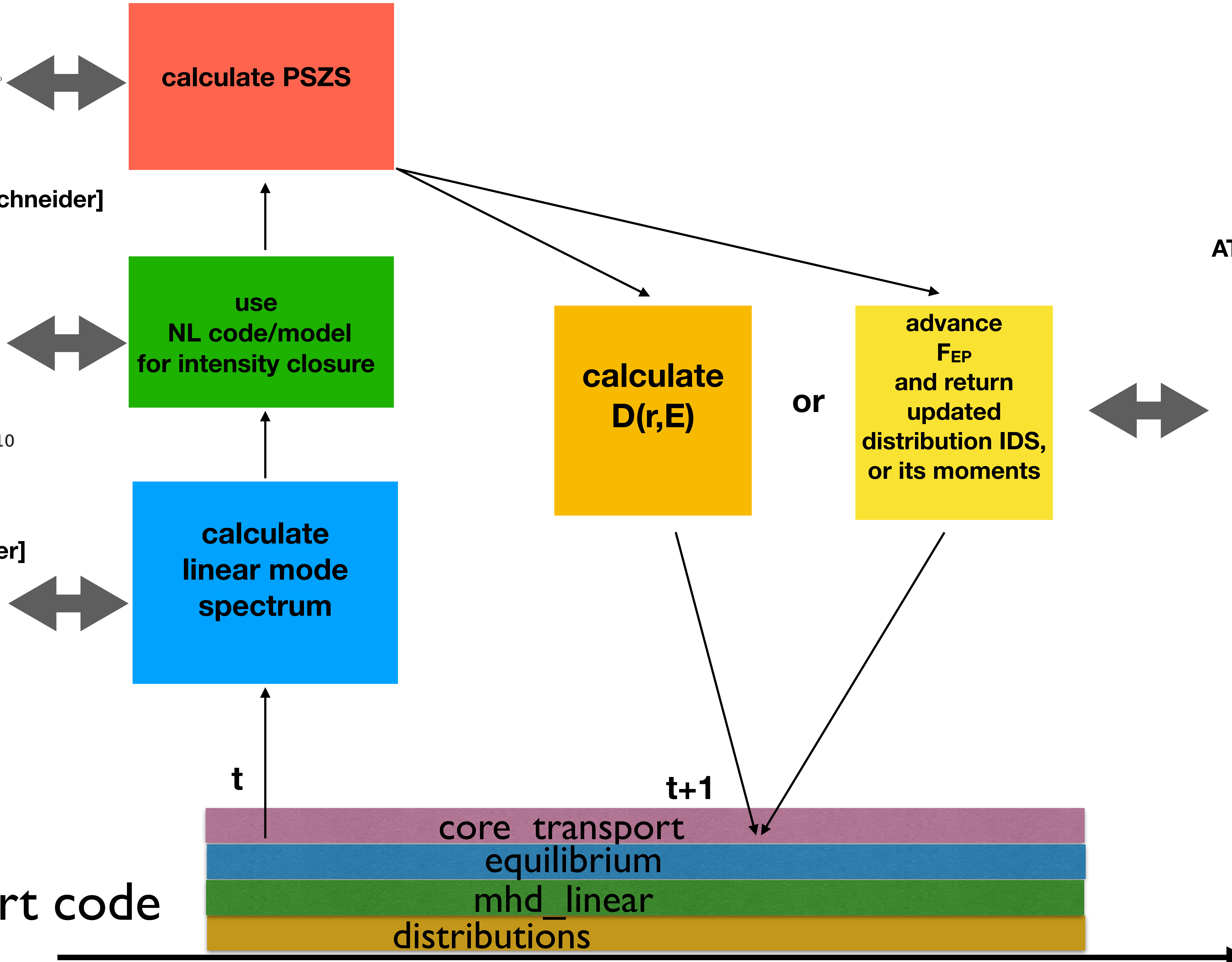


[HAGIS, S.D. Pinches, T Hayward-Schneider]

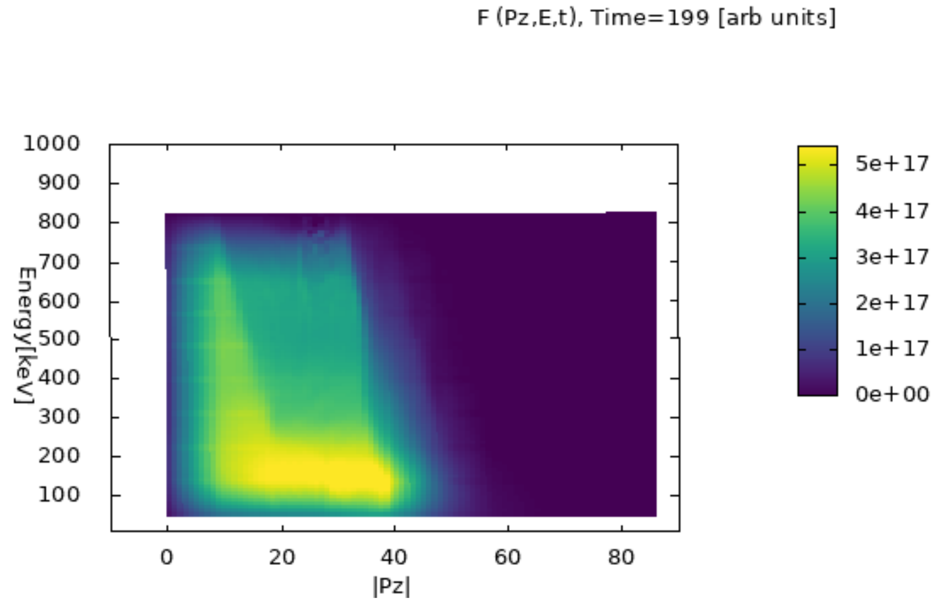


EP WF (LIGKA) [A . Popa, Ph. Lauber]





ATEP code [Ph. Lauber, 2022]



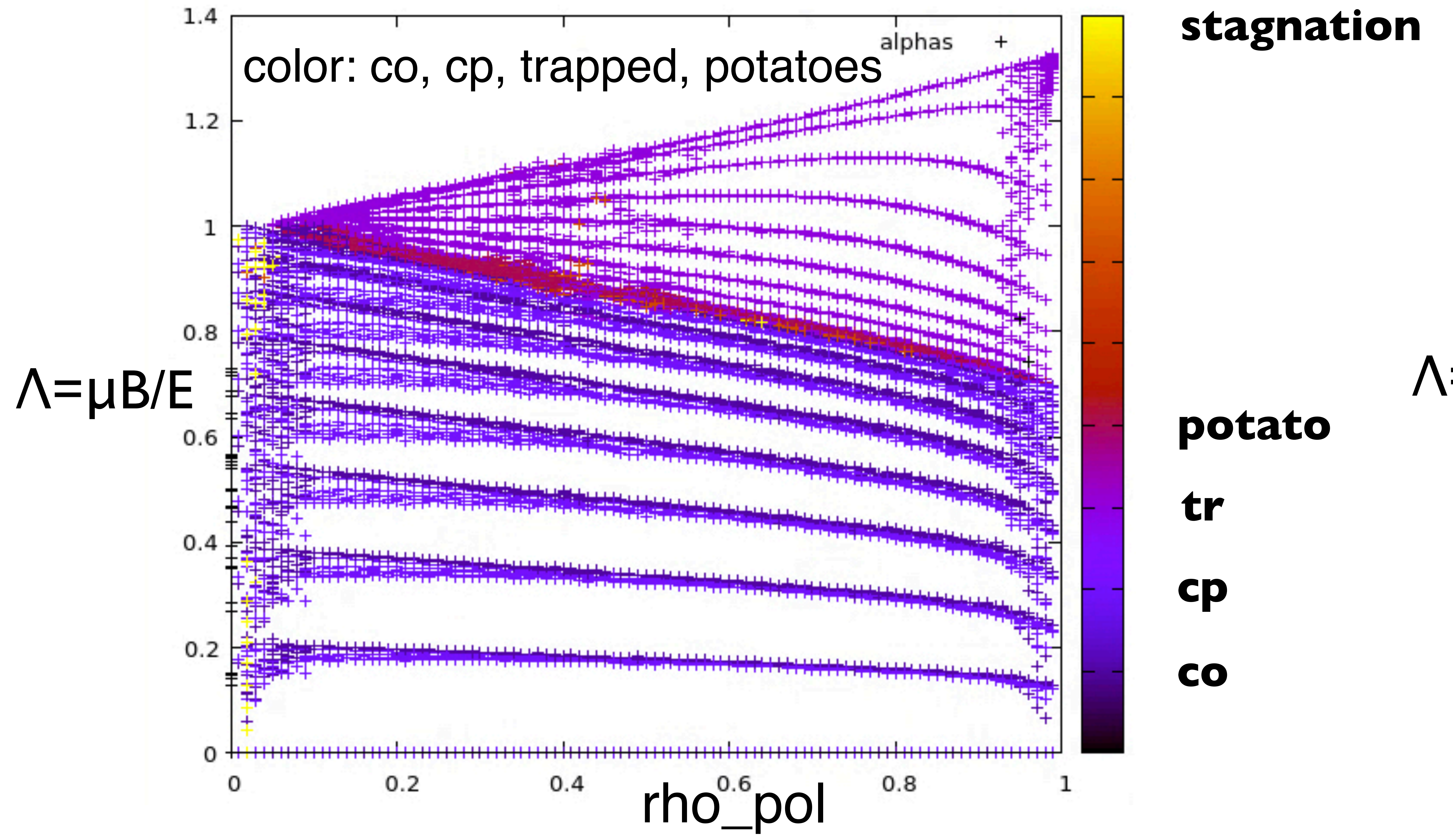
$$\frac{\partial F_{EP}}{\partial t} = \frac{\partial Pz}{\partial t}\frac{\partial F_{EP}}{\partial P_z} + \frac{\partial E}{\partial t}\frac{\partial F_{EP}}{\partial E}$$

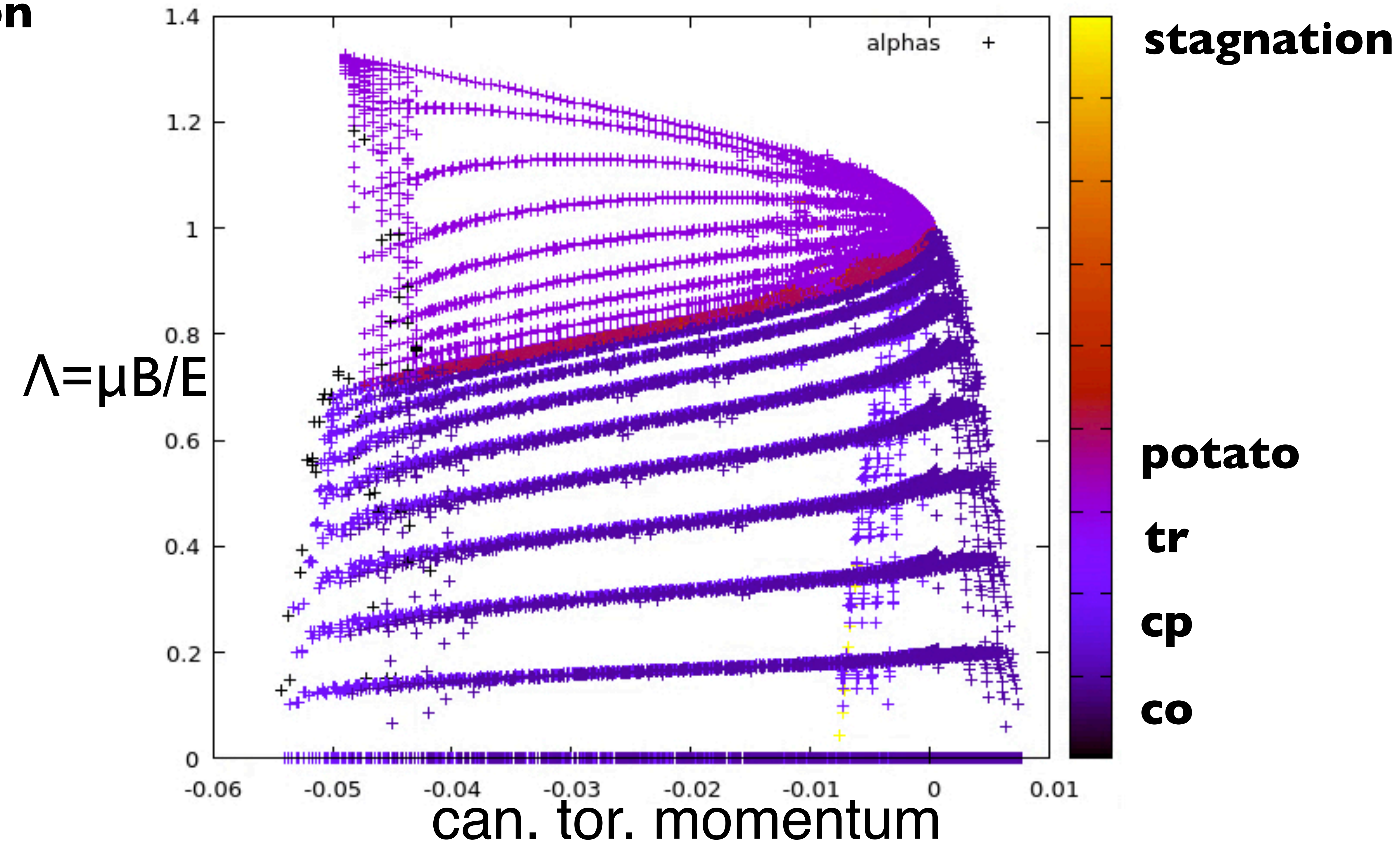
calculating PSZSs

calculating PSZS using FINDER/HAGIS

- use LIGKA related code **FINDER** to set up marker space, determine trapped-passing boundary, sort, classify, orbit averages for unperturbed equilibria
- originally developed to calculate propagator integrals for LIGKA
- now updated and ported to IMAS
- add perturbation, as originally implemented in HAGIS model [S.D. Pinches 1998]

[A. Bierwage, CPC 2022, LIGKA orbit integrals, CPC 2007]



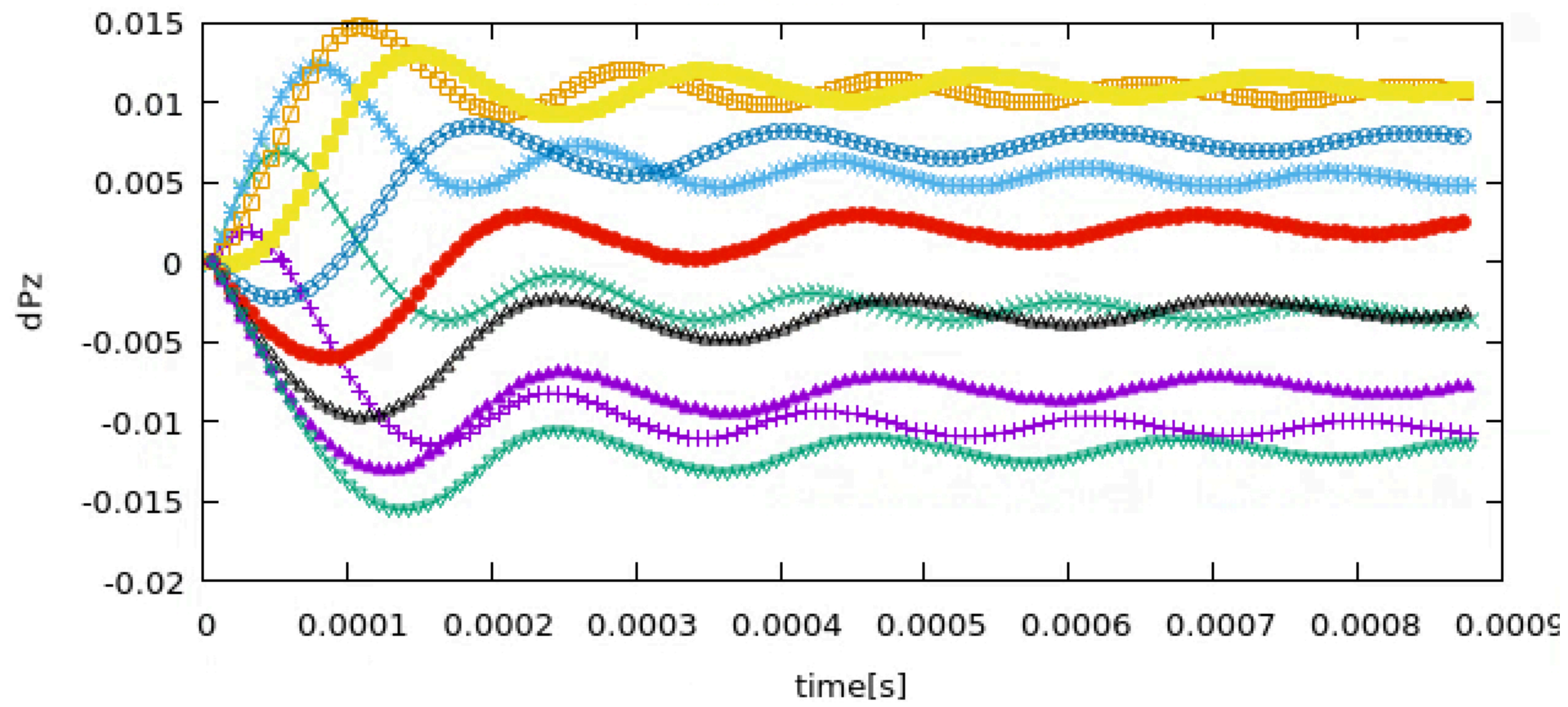


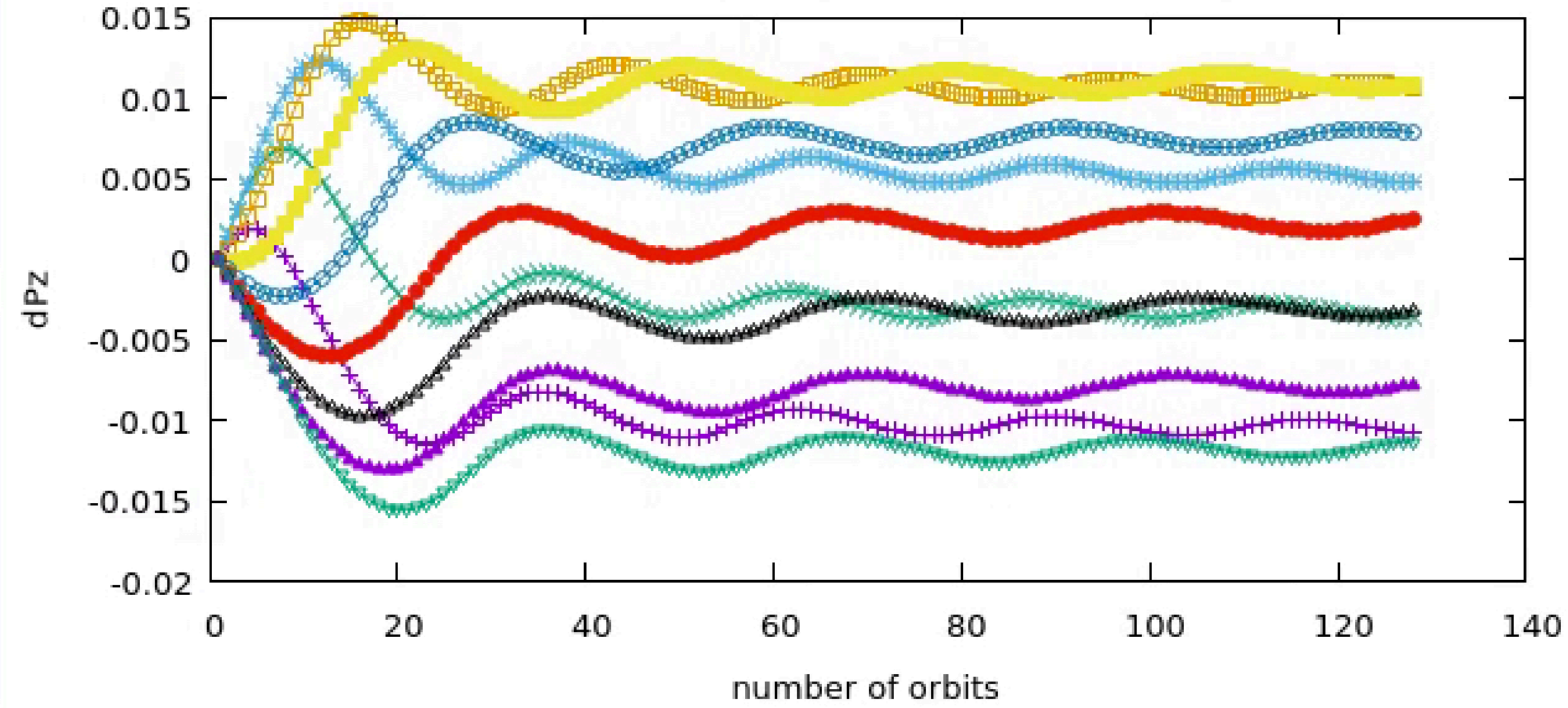
- distributions IDS holds all orbit-averaged information about marker space
- fast, repetitive calls of HAGIS library within IMAS are possible - **mapping between Pz and <radial position>**!
- extended IDS structures were needed, MDS+ limitations (2GB) avoided by moving to HDF5 backend

calculating PSZS using FINDER/HAGIS

adding LIGKA calculated perturbation: follow set of market for wave-periods, time or number of orbits

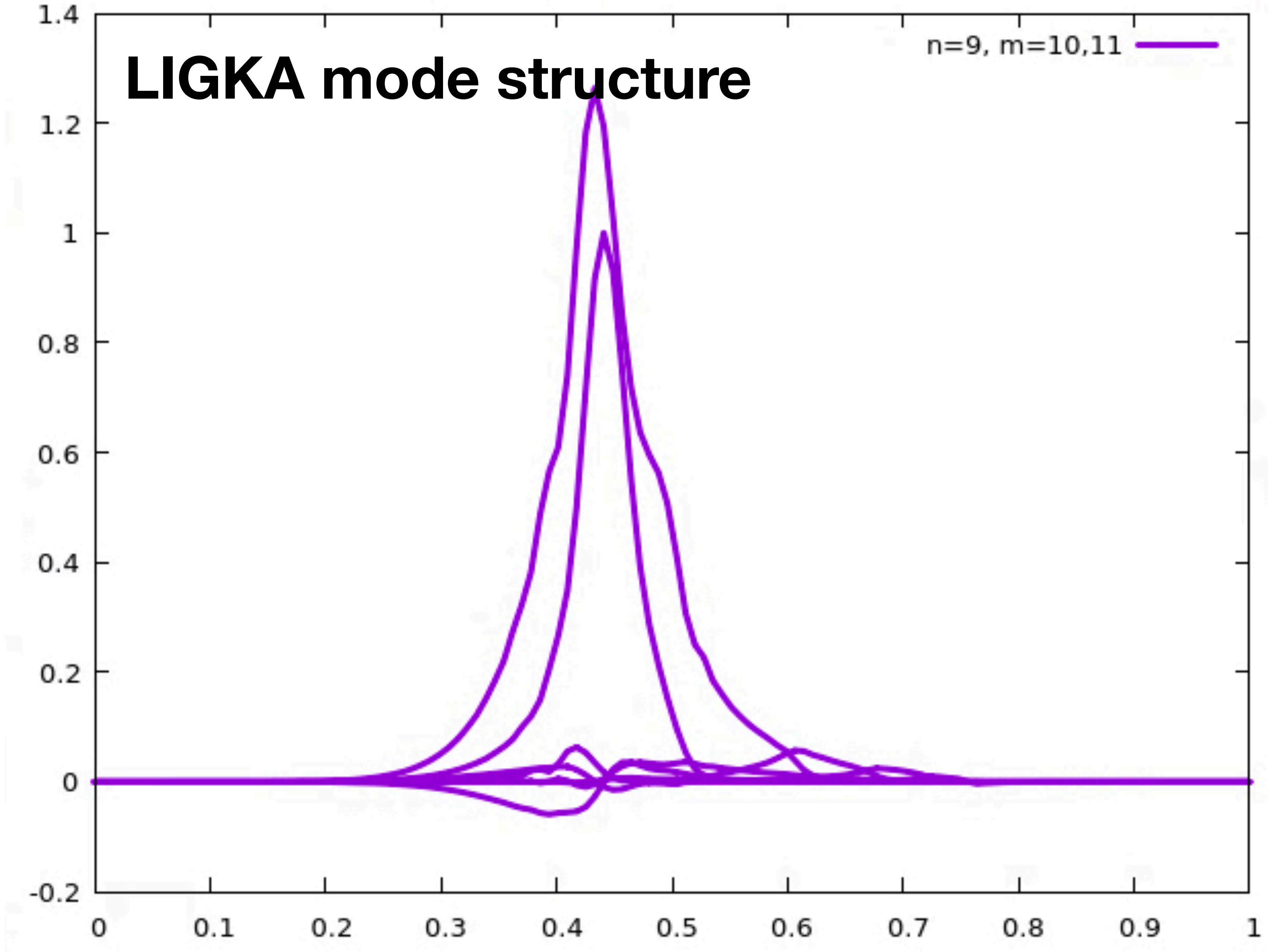
mid-radius, 1 MeV, He, co-passing, Λ=0, n=9 TAE with dB/B=10^{-3}





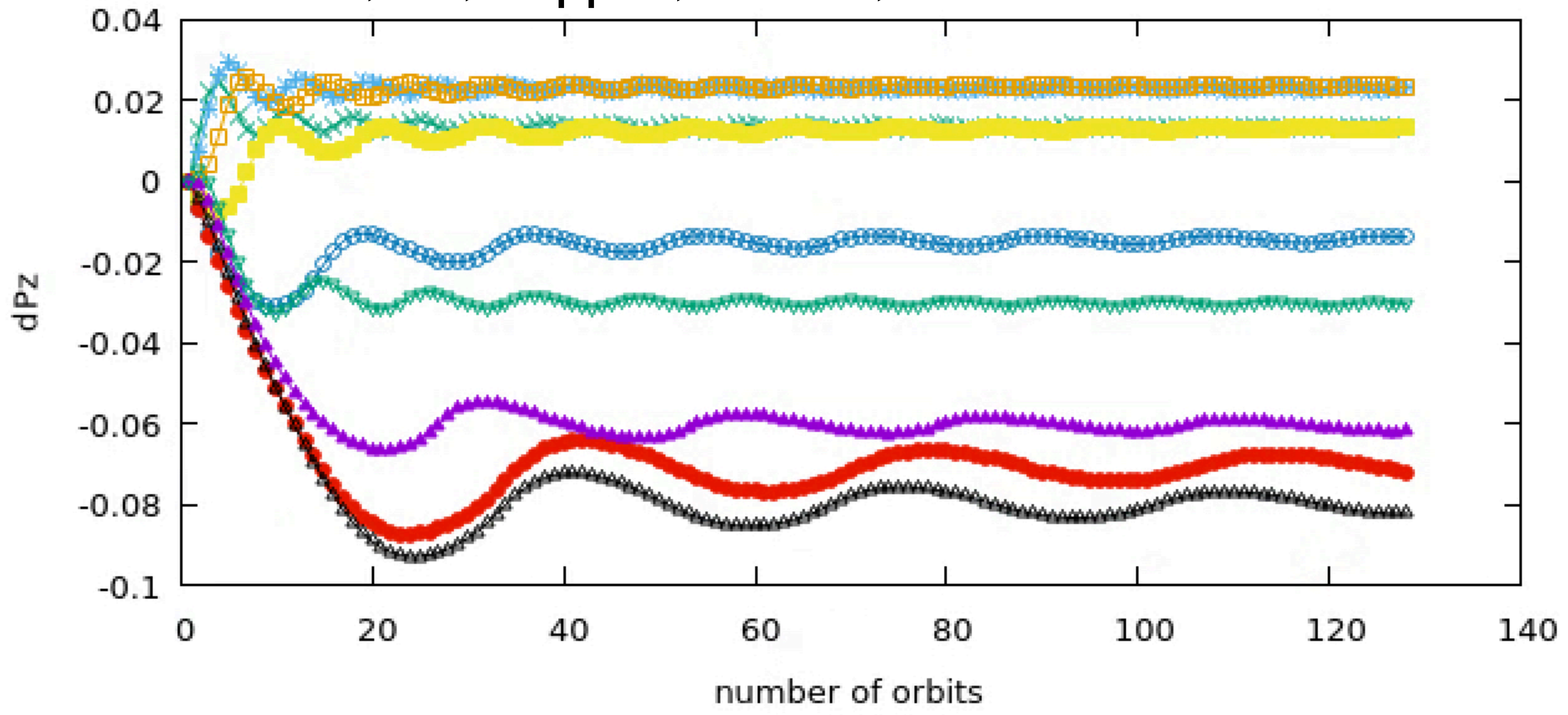
colours: different starting phase, 10 markers with starting tor. angle [0: 2π/n]

important: averaging over phase is crucial to obtain correct fluxes



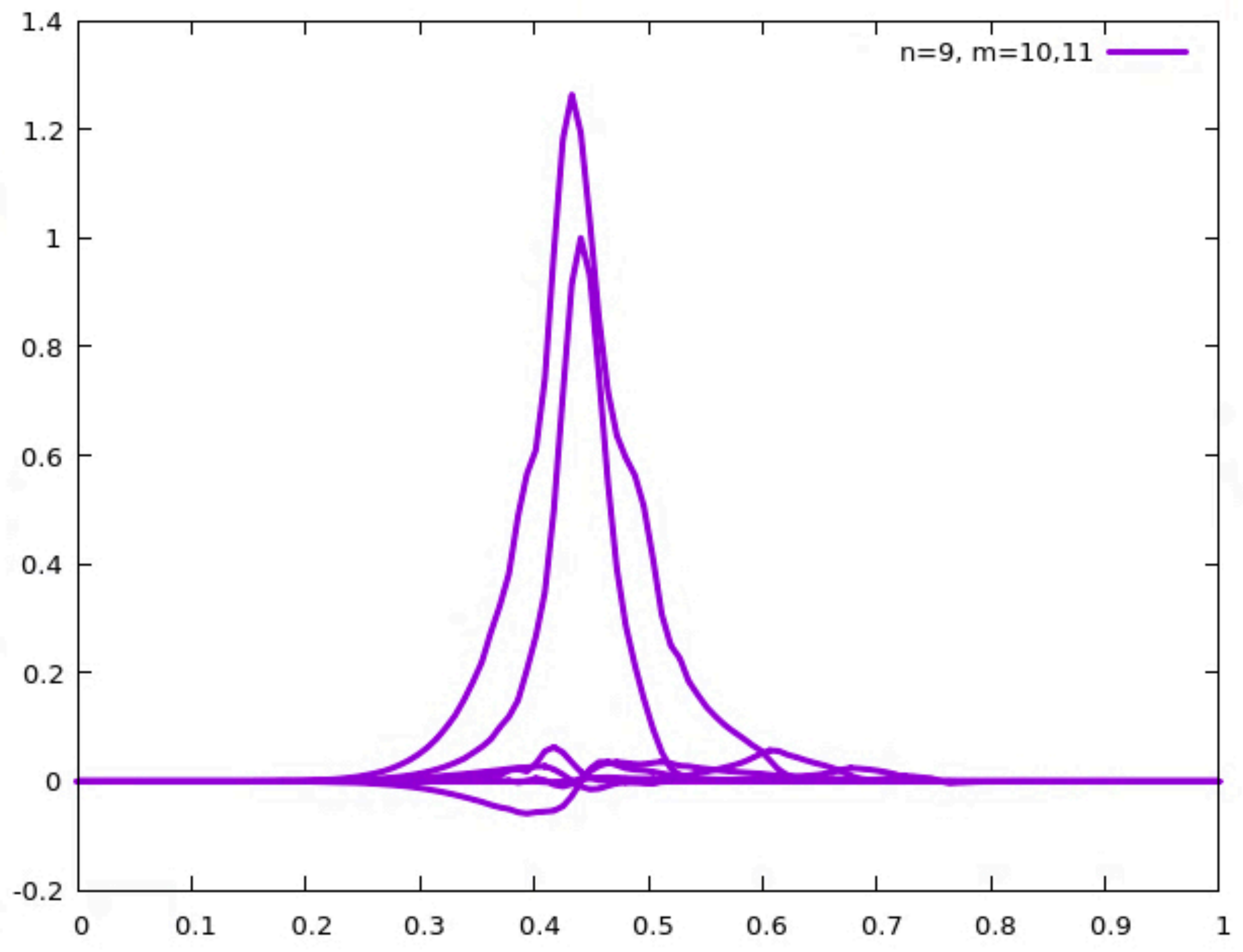
calculating PSZS using FINDER/HAGIS

1 MeV, He, trapped, Λ=1.03, n=9 TAE with $dB/B=10^{-3}$

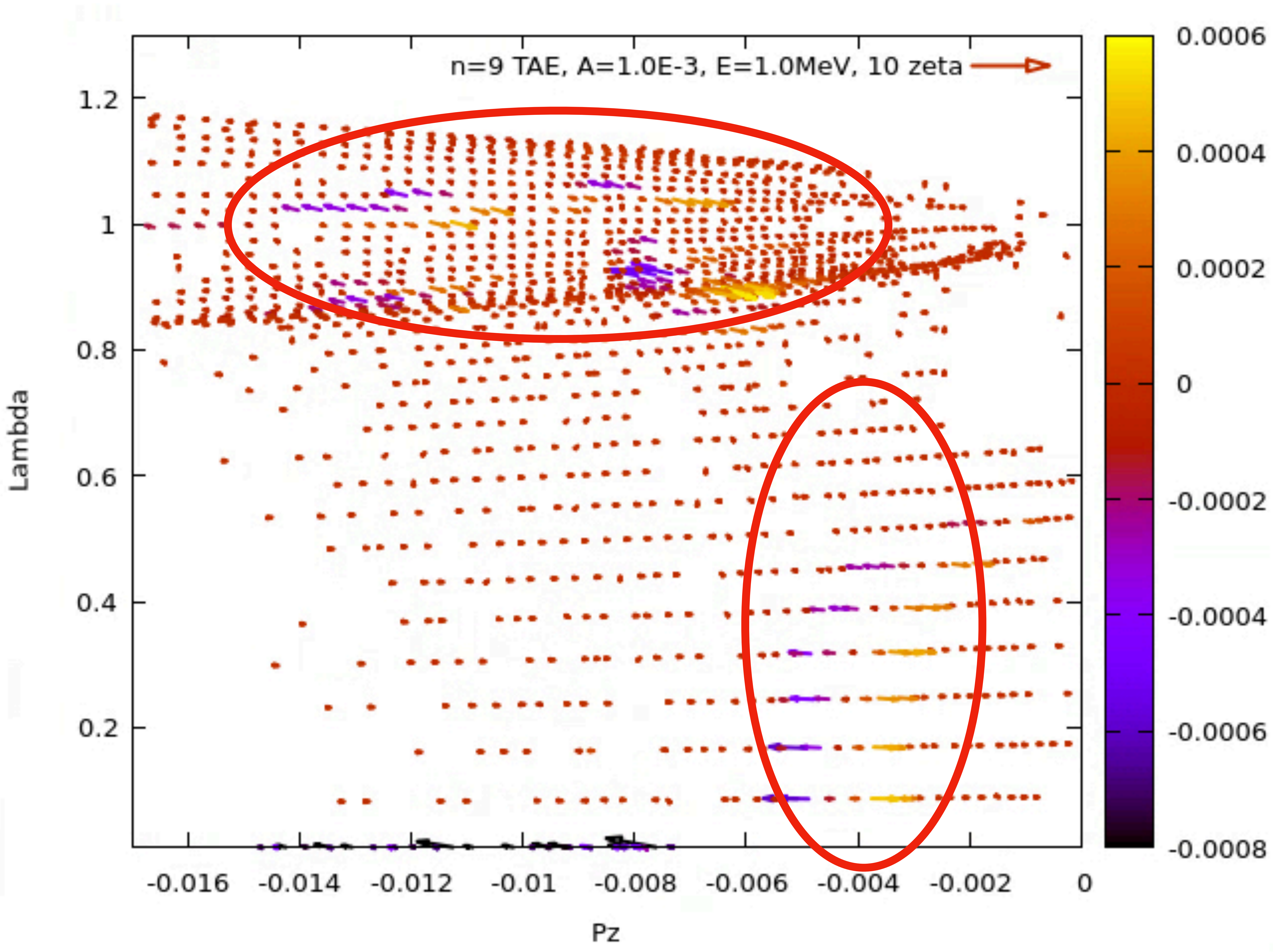


averaging over markers with different phase gives effective poloidally and toroidally averaged dPz

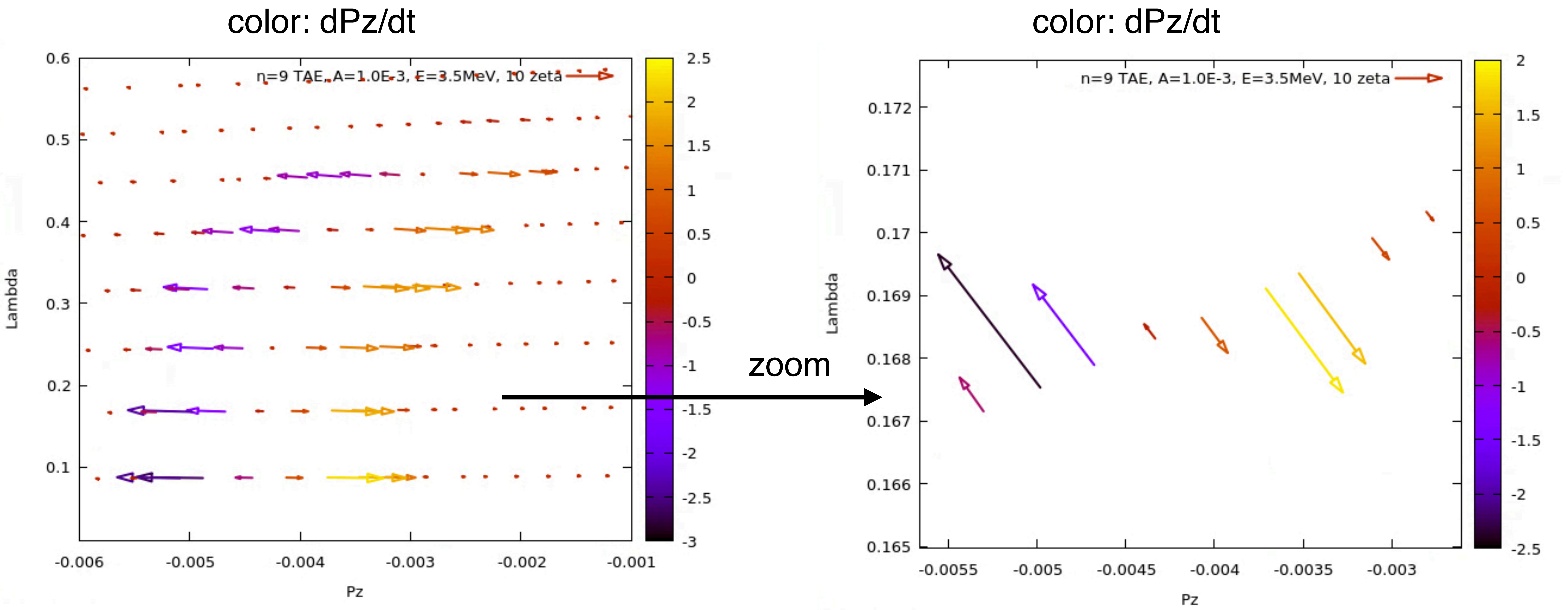
what is dPz, dE, dΛ for given perturbation after x completed orbits?



- arrows: initial (Pz,Λ) → (Pz+δPz,Λ+δΛ)
- color: δPz
- averages over 10 phases, 64 orbits
- 2-5 minutes to calculate
- modular structure of FINDER allows to replace HAGIS with newer/faster code of same functionality



calculate fluxes: dPz/dt [(eV/s)/s]



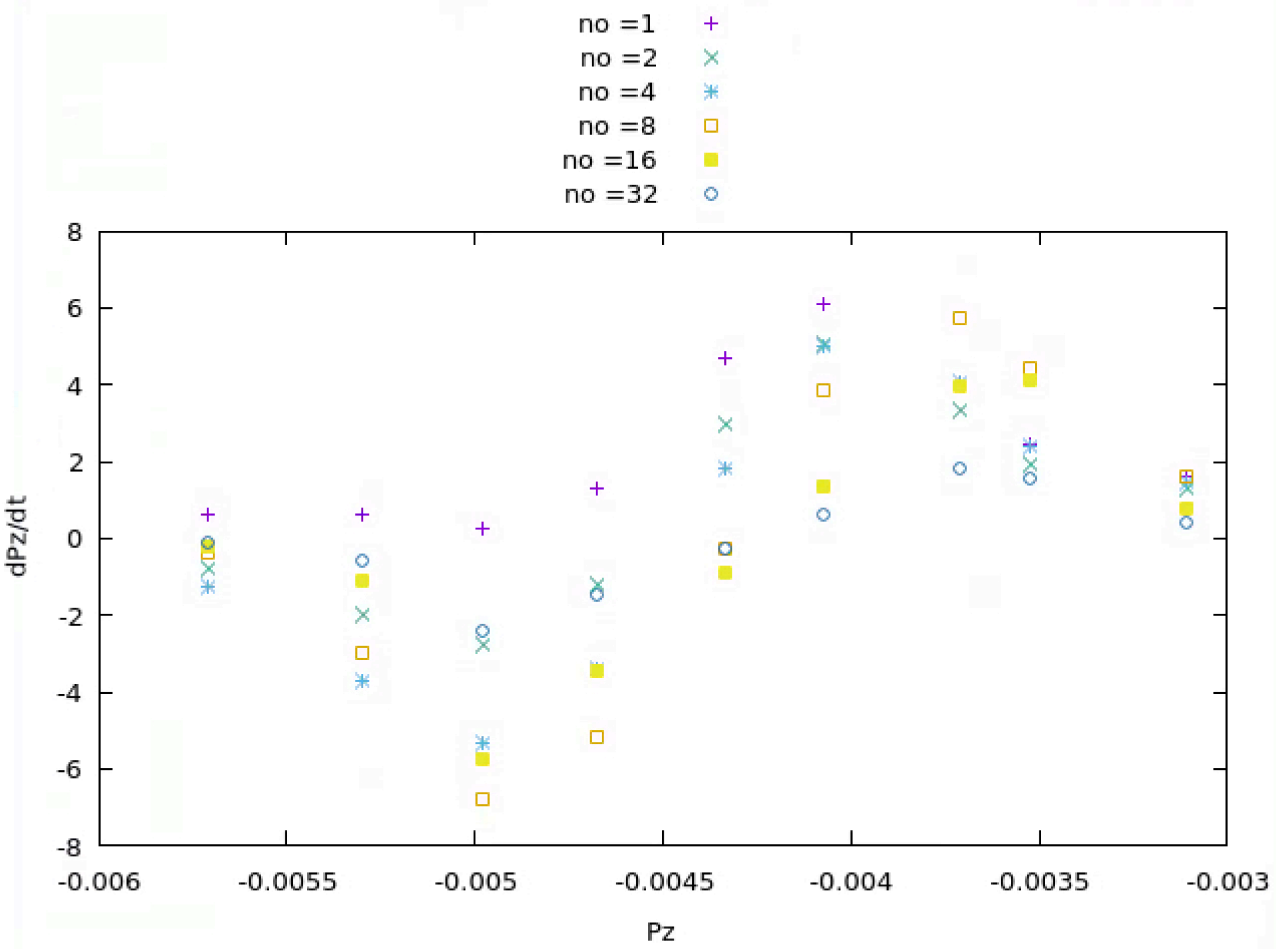
- divide δPz by orbit transit time and number of orbits (here 32)
- the same information is available for Λ and E
- transport coefficients $D_{Pz}=(dPz)^2/dt$ and $K_{Pz}=(dPz)/dt$ can be evaluated

how many orbits we need to follow in presence of perturbation?

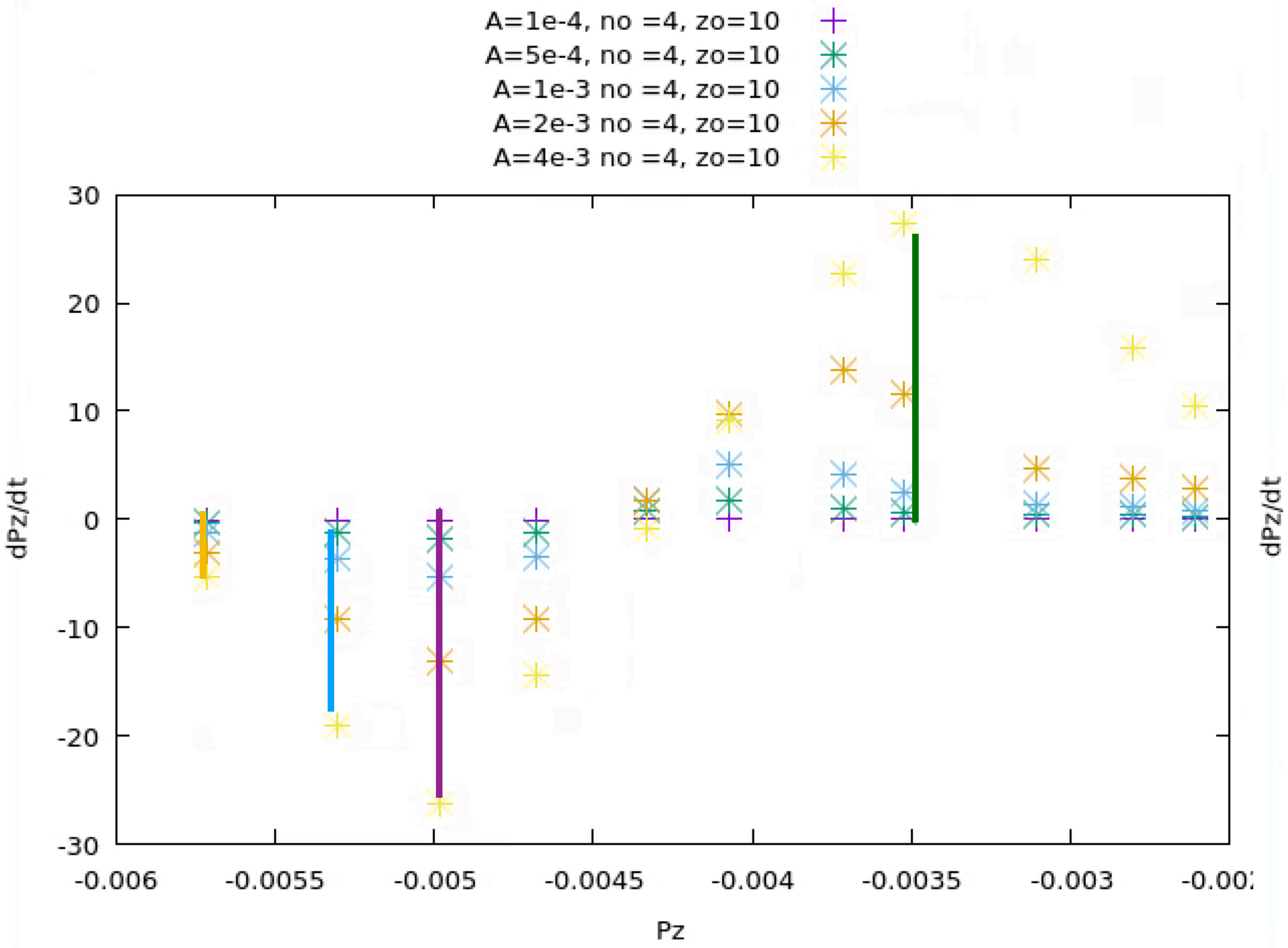
depending on what type of problem is to be solved (shortest time scale to be resolved), very few orbit transits (4-8) are sufficient.

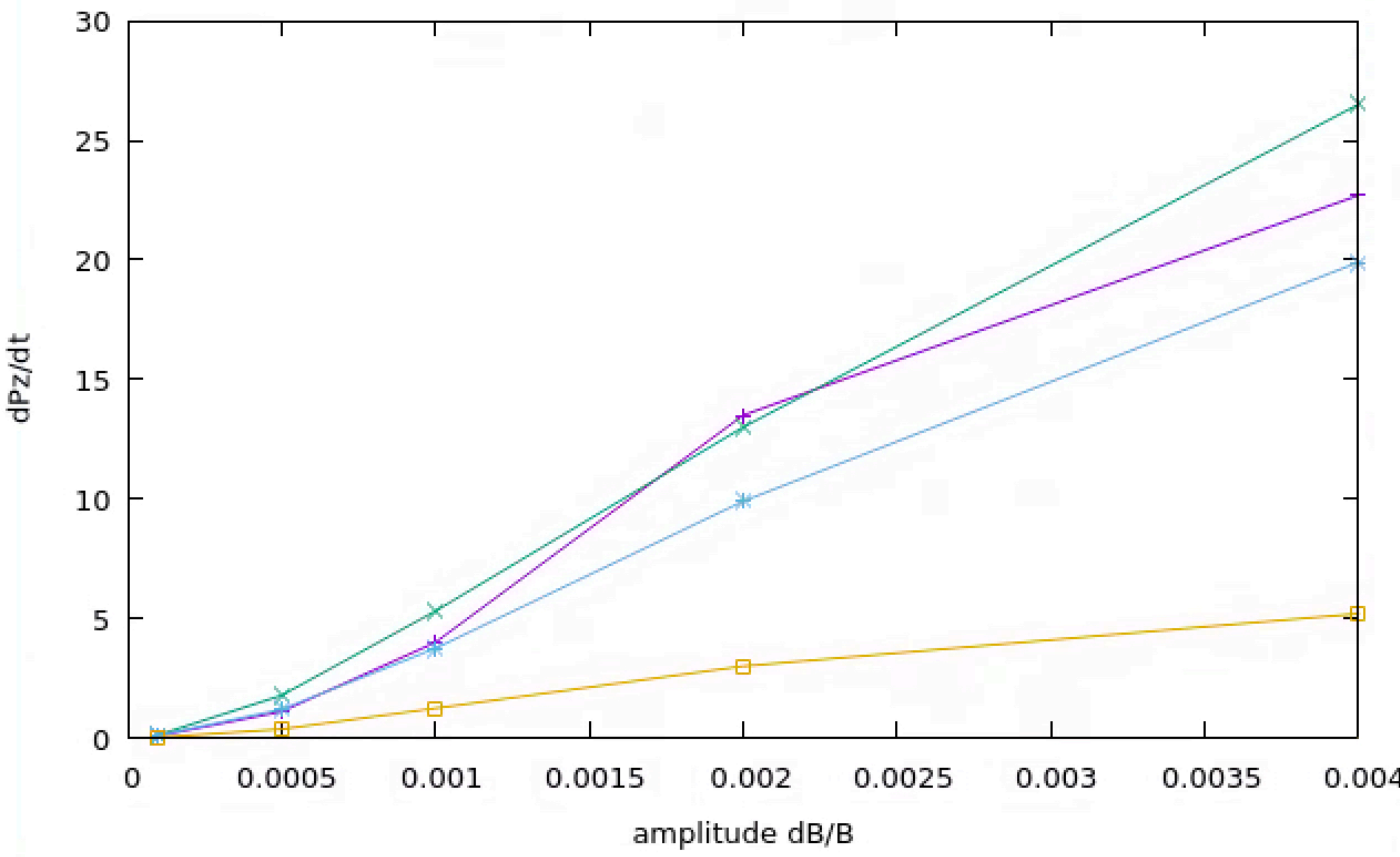
physics reason:

- resonance conditions 'selects' particles that suffer transport
- nth-order resonance is covered after n orbits
- 5-10 poloidal orbits typically cover also precessional resonance for many AEs
- also non-resonant transport is sufficiently represented after 10 orbits (note, that we follow markers for fixed number of orbits, not total time!)
- cases with very large amplitude where Pz-transport saturation occurs in a few poloidal orbits might need adoption of parameters



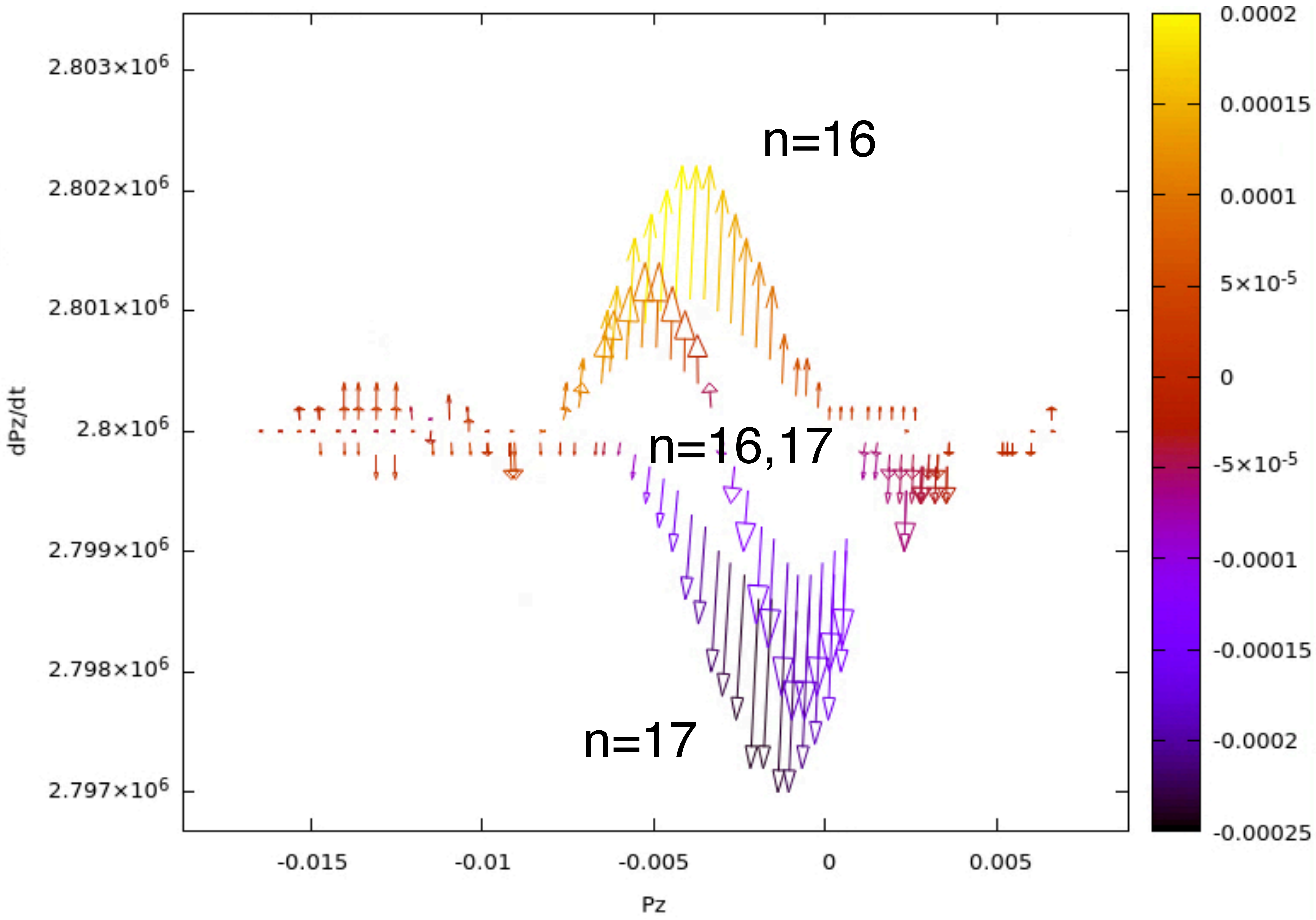
amplitude dependence: dB/B =[10^{-4} - $4 \cdot 10^{-3}$]





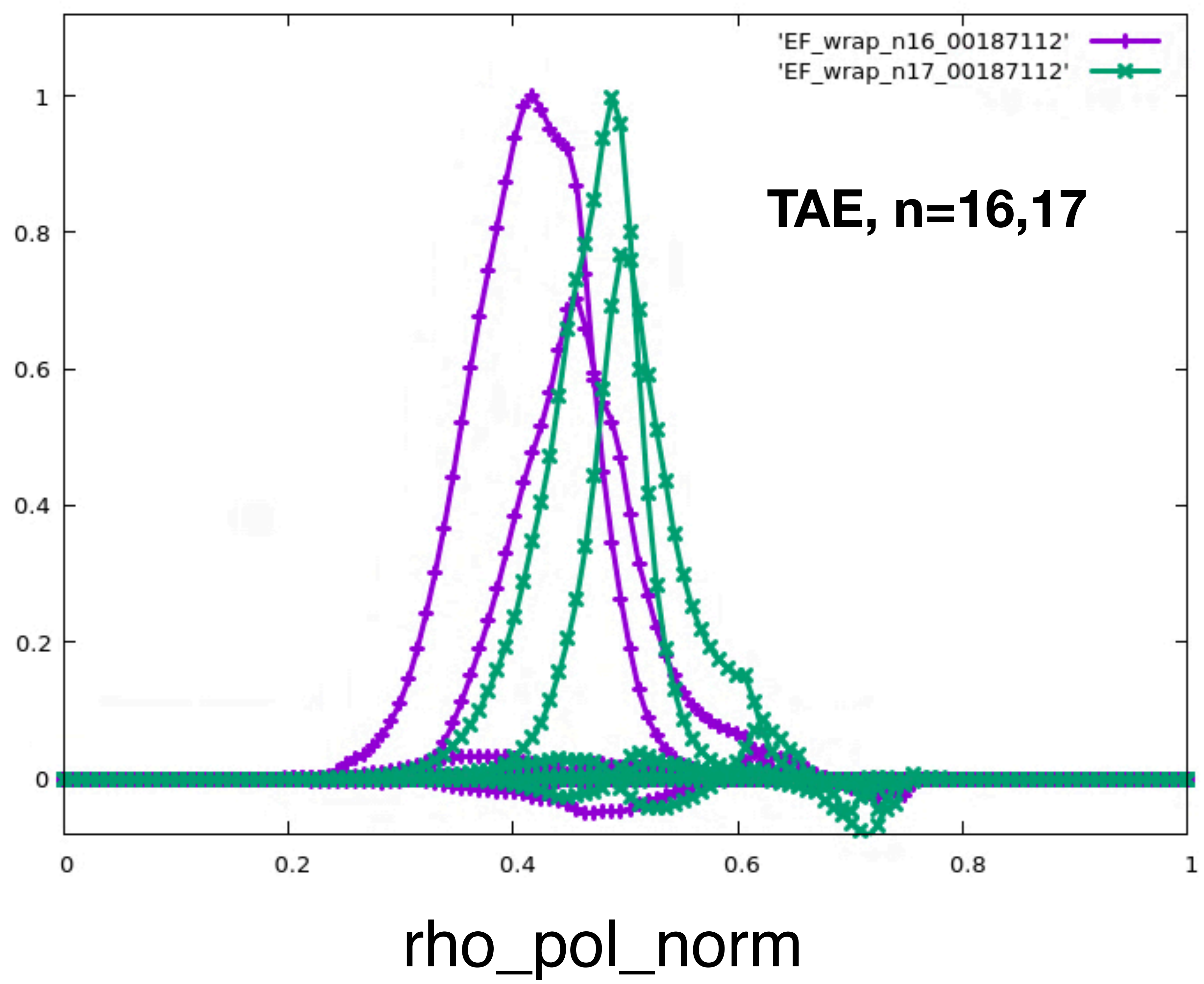
- dPz/dt ~ quadratic for small amplitudes, linear for larger amplitudes
- simple interpolation captures the amplitude scaling

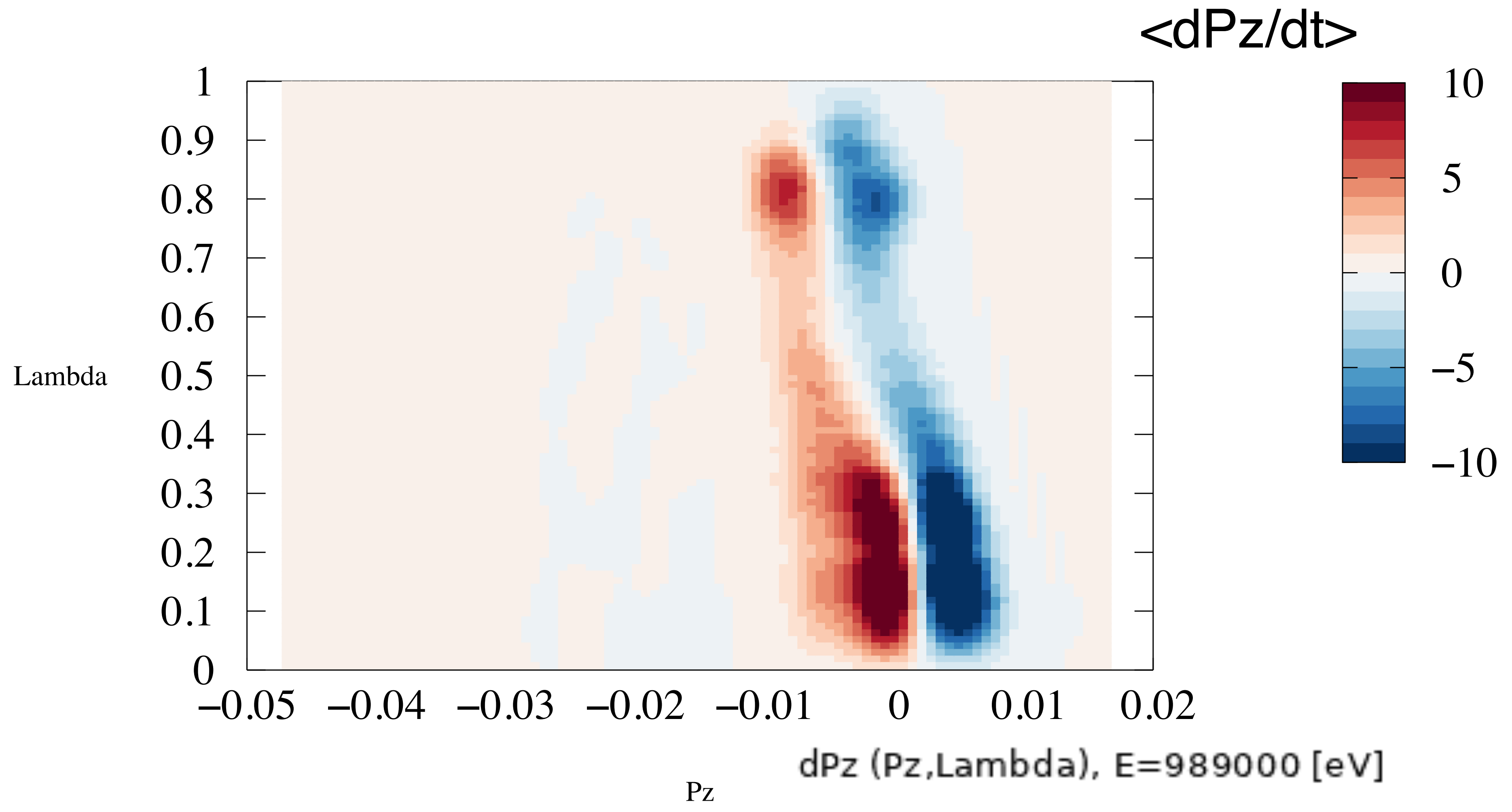
easy to include more than one perturbation:



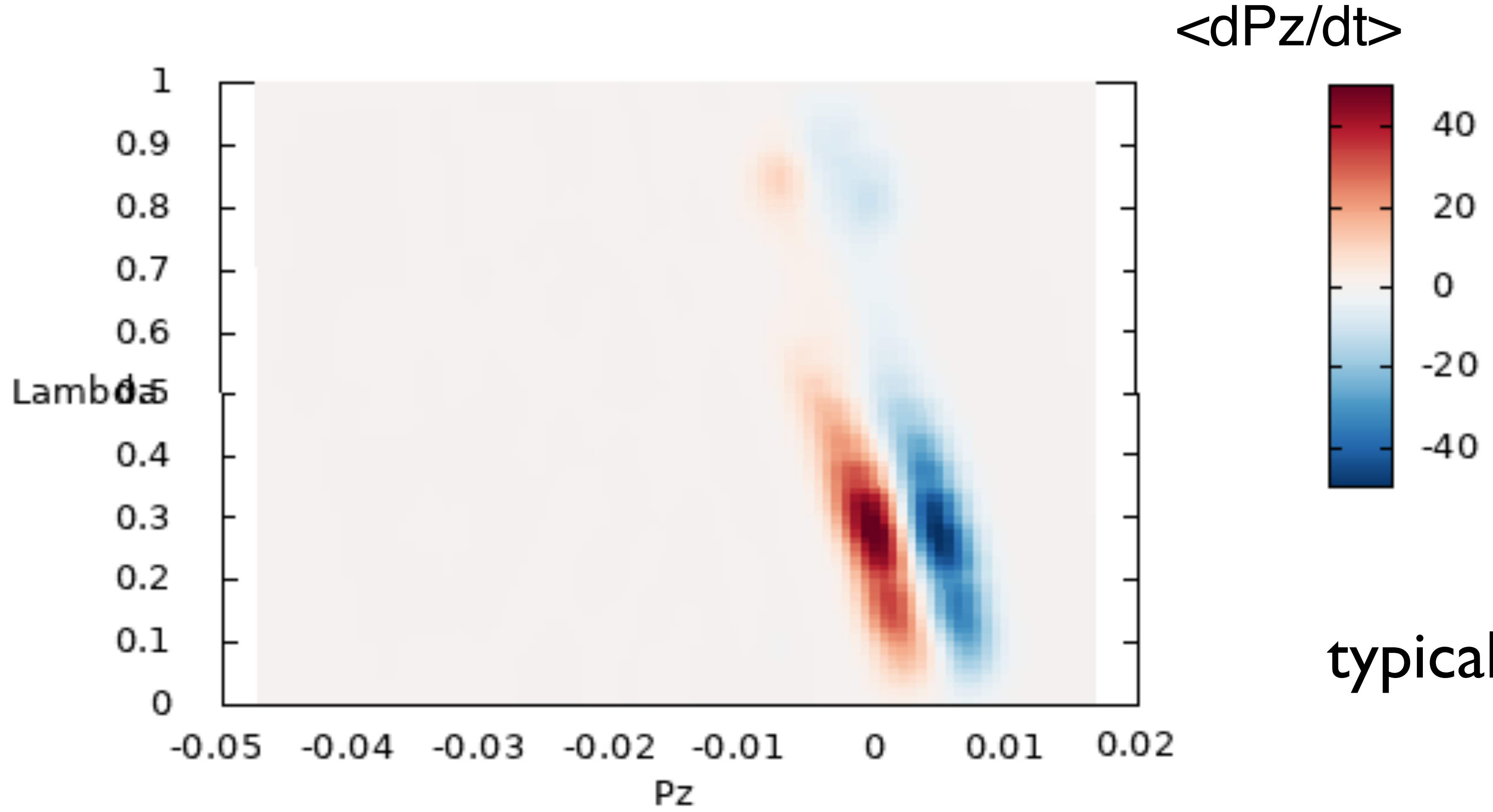
implementation details: example ITER 100015,1

- calculate <dPz/dt> , <dE/dt> for given fixed mode structures at fixed amplitude with FINDER/HAGIS, write into IDS (dB/B=5*10^{-3})
- ATEP code: read FINDER data, use 3D bspline methods to create <dPz/dt> , <dE/dt> on 3D grid as F_{EP}
- use 3d scattered-data b-spline algorithm [Scattered Data Interpolation with Multilevel B-Splines, Lee 1997] - post-smoothing may be still implemented





co-passing particles



typical grid: (Pz,E,Λ) (128x40x40)

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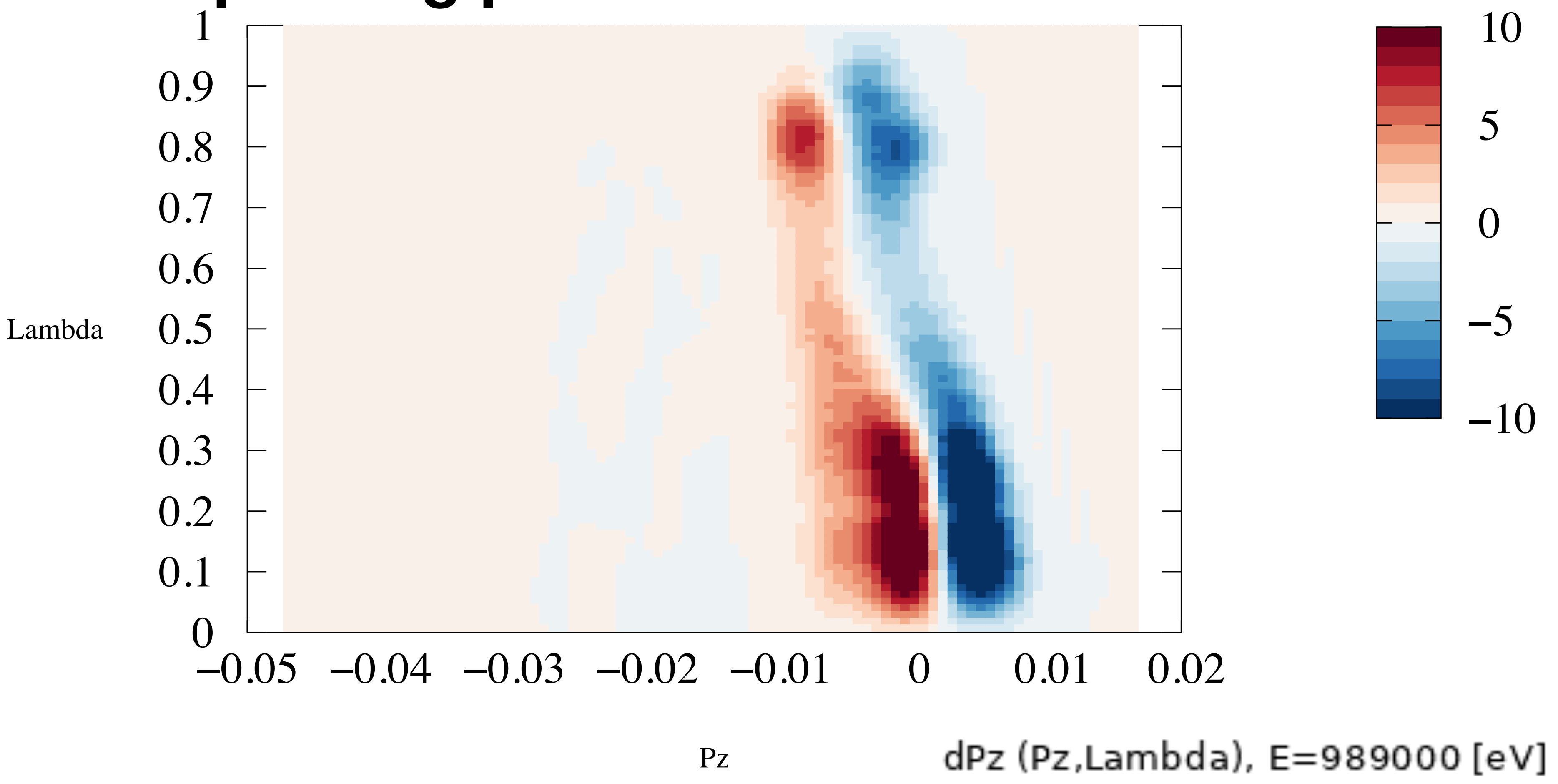
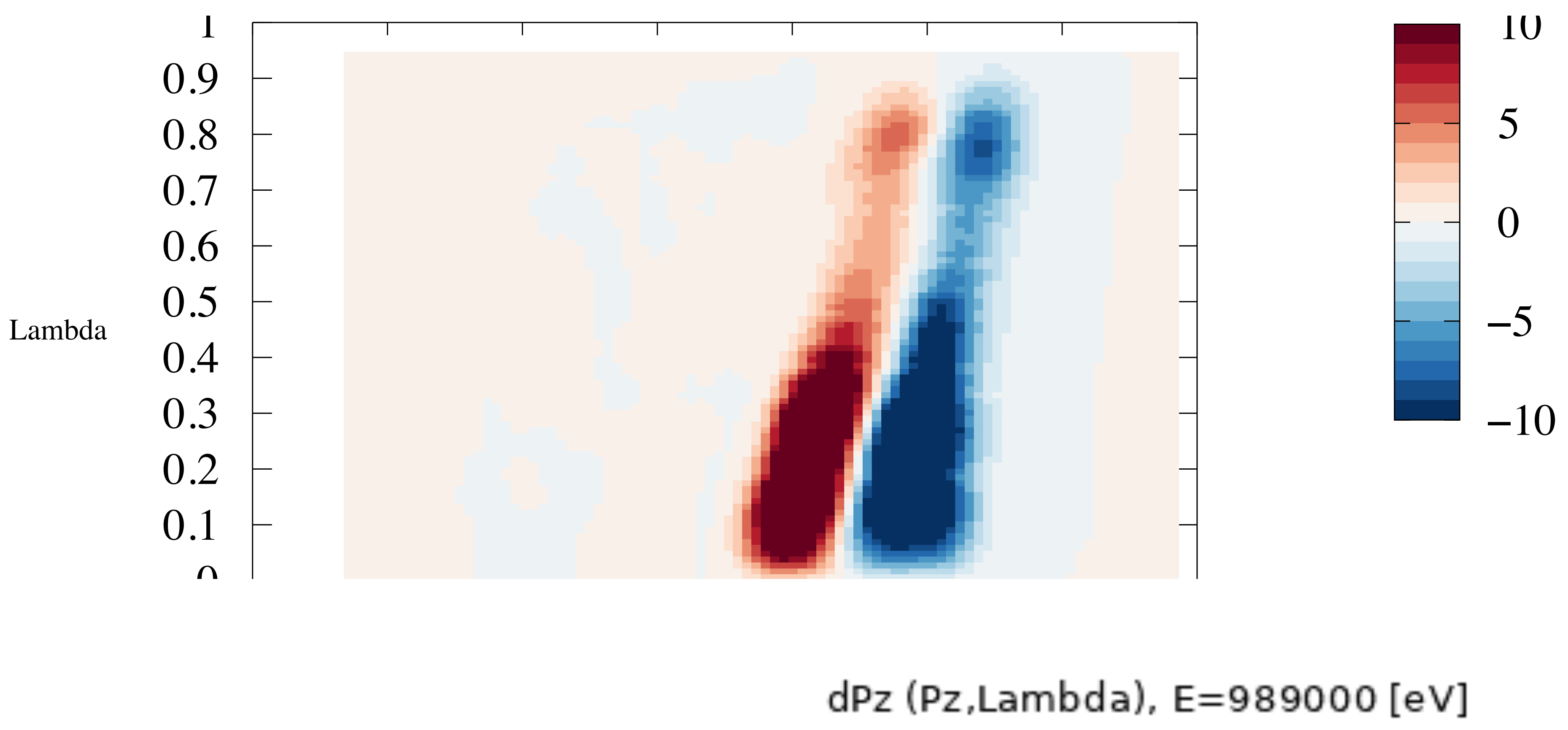
co-passing particles

<dPz/dt>

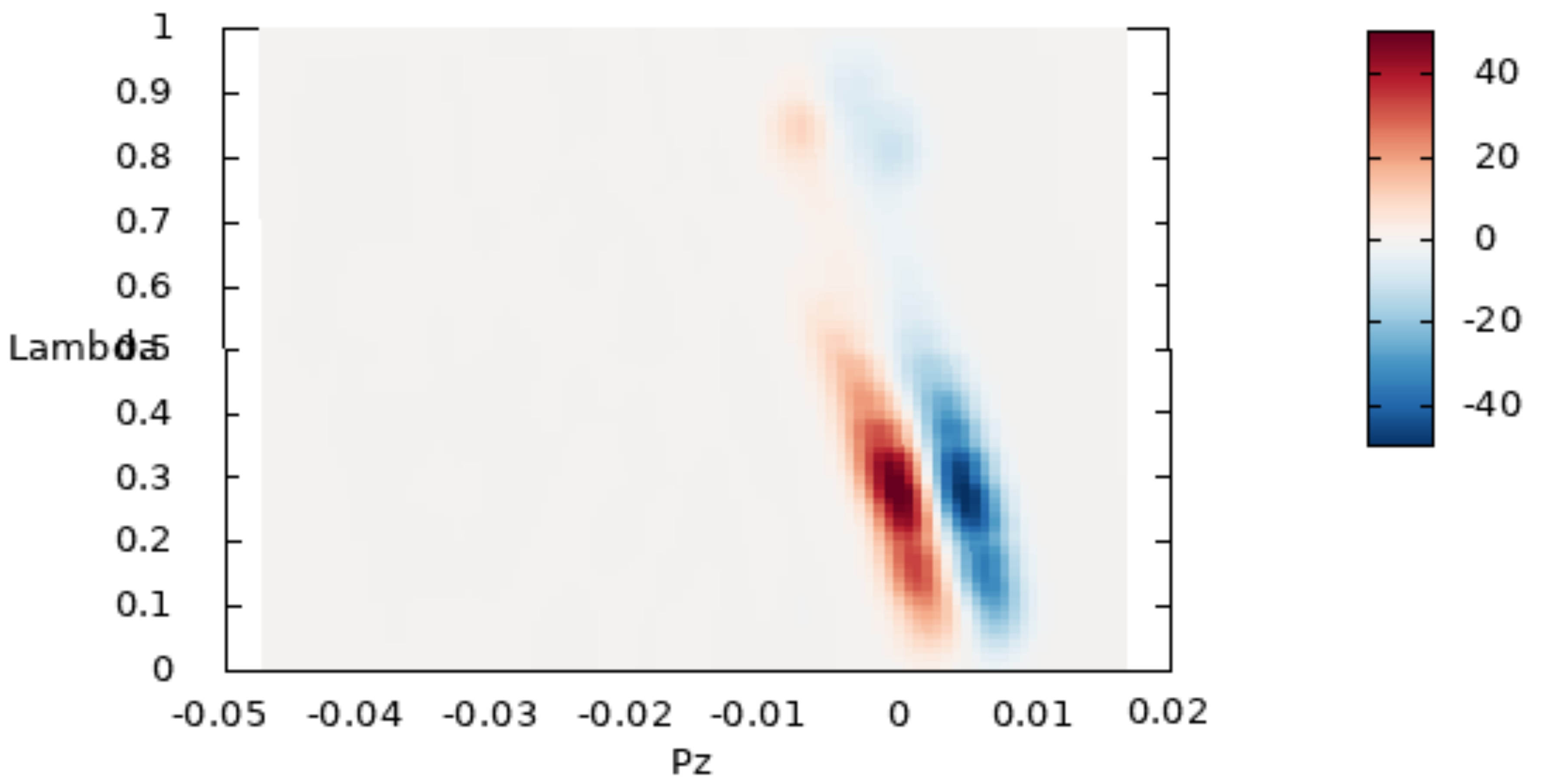


counter-passing particles

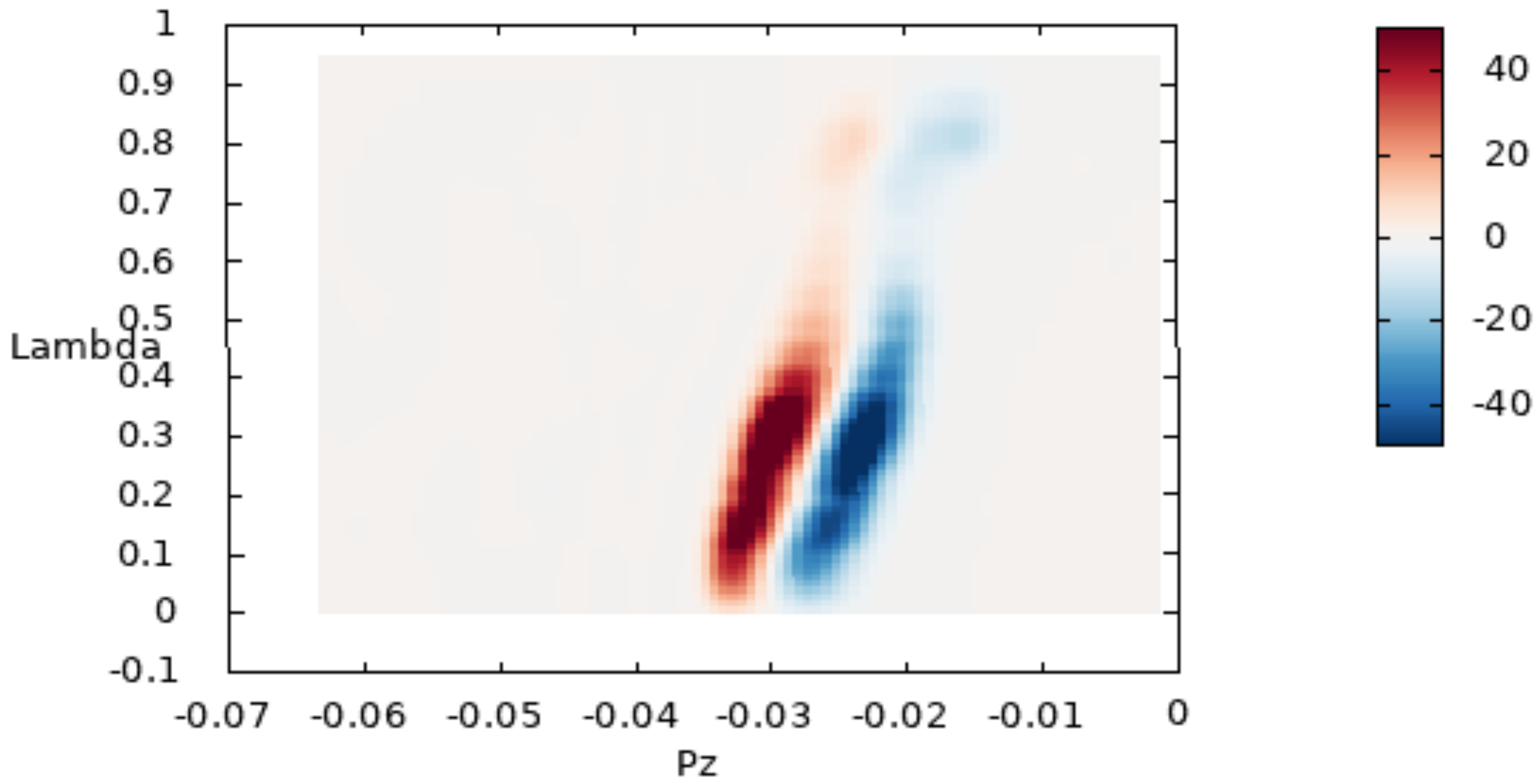
<dPz/dt>



<dPz/dt>



<dPz/dt>



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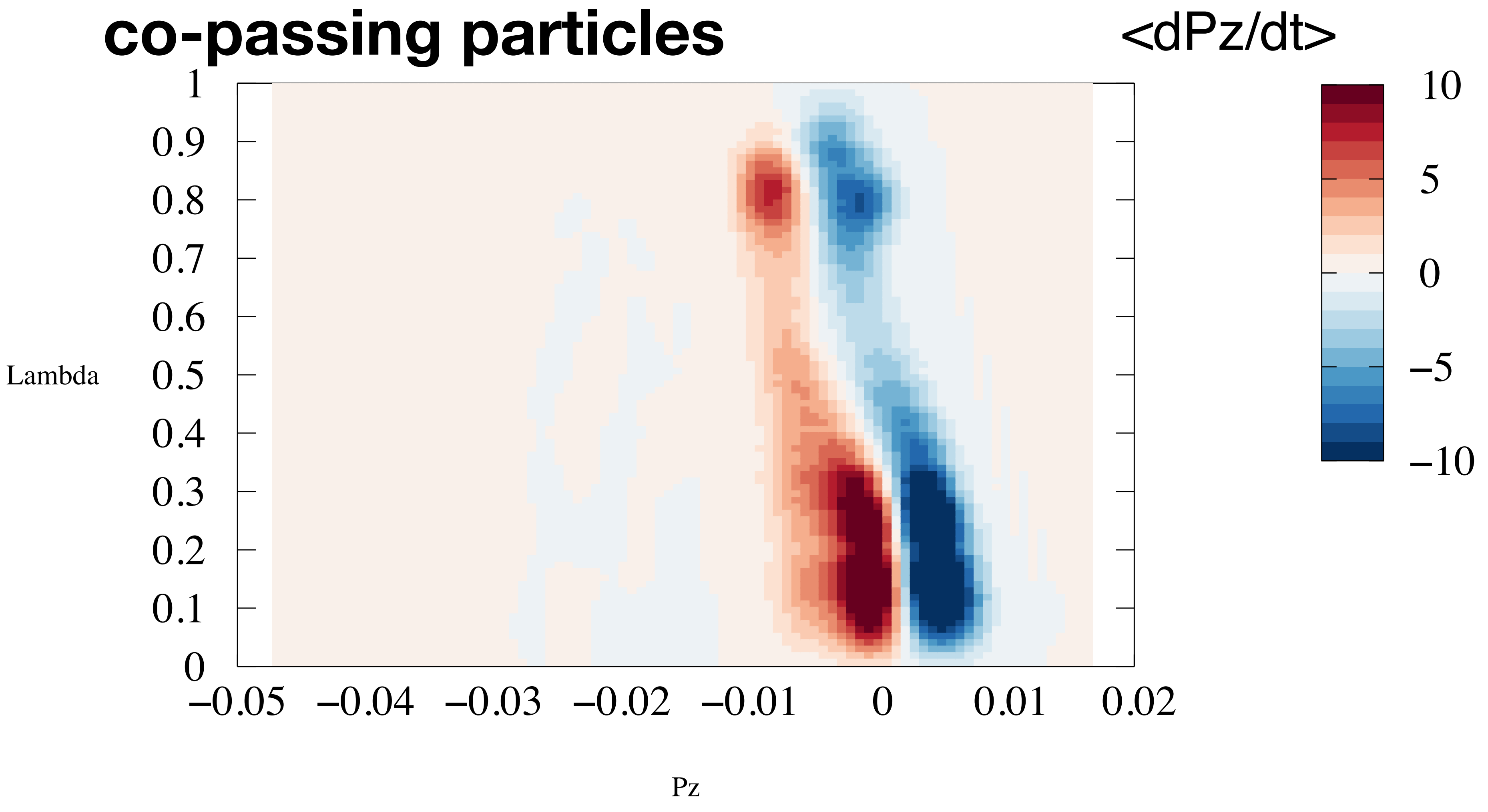
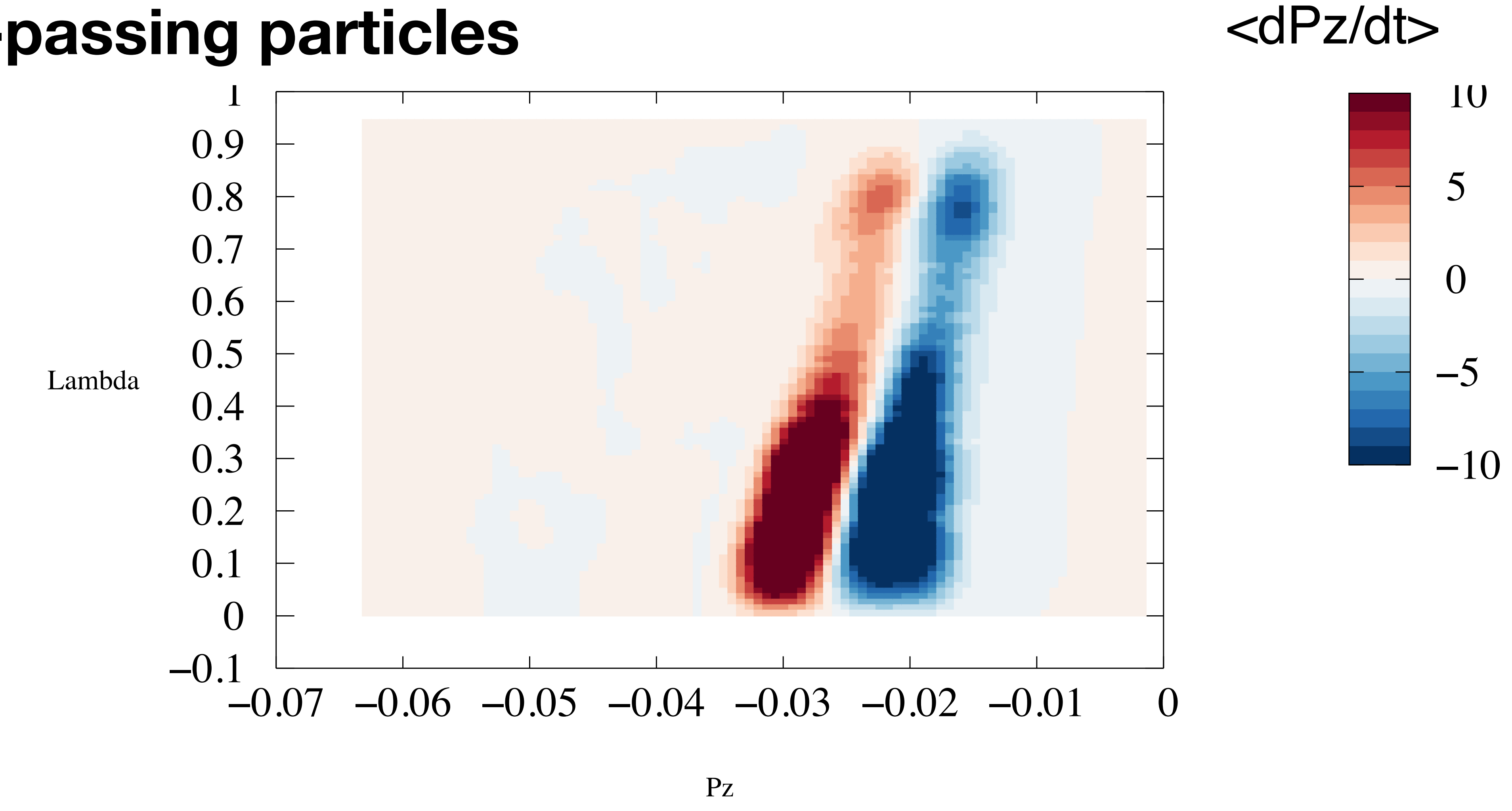
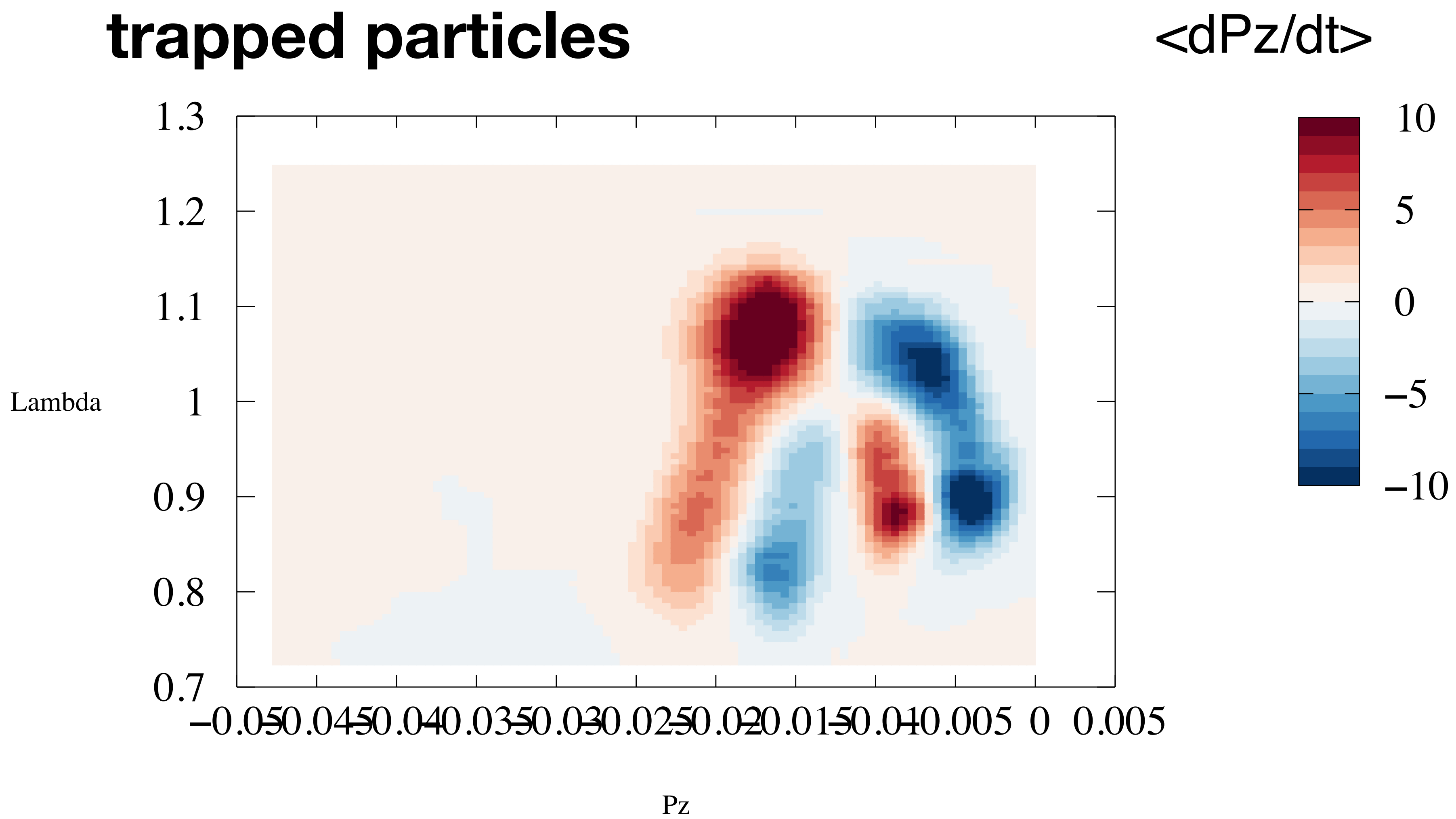


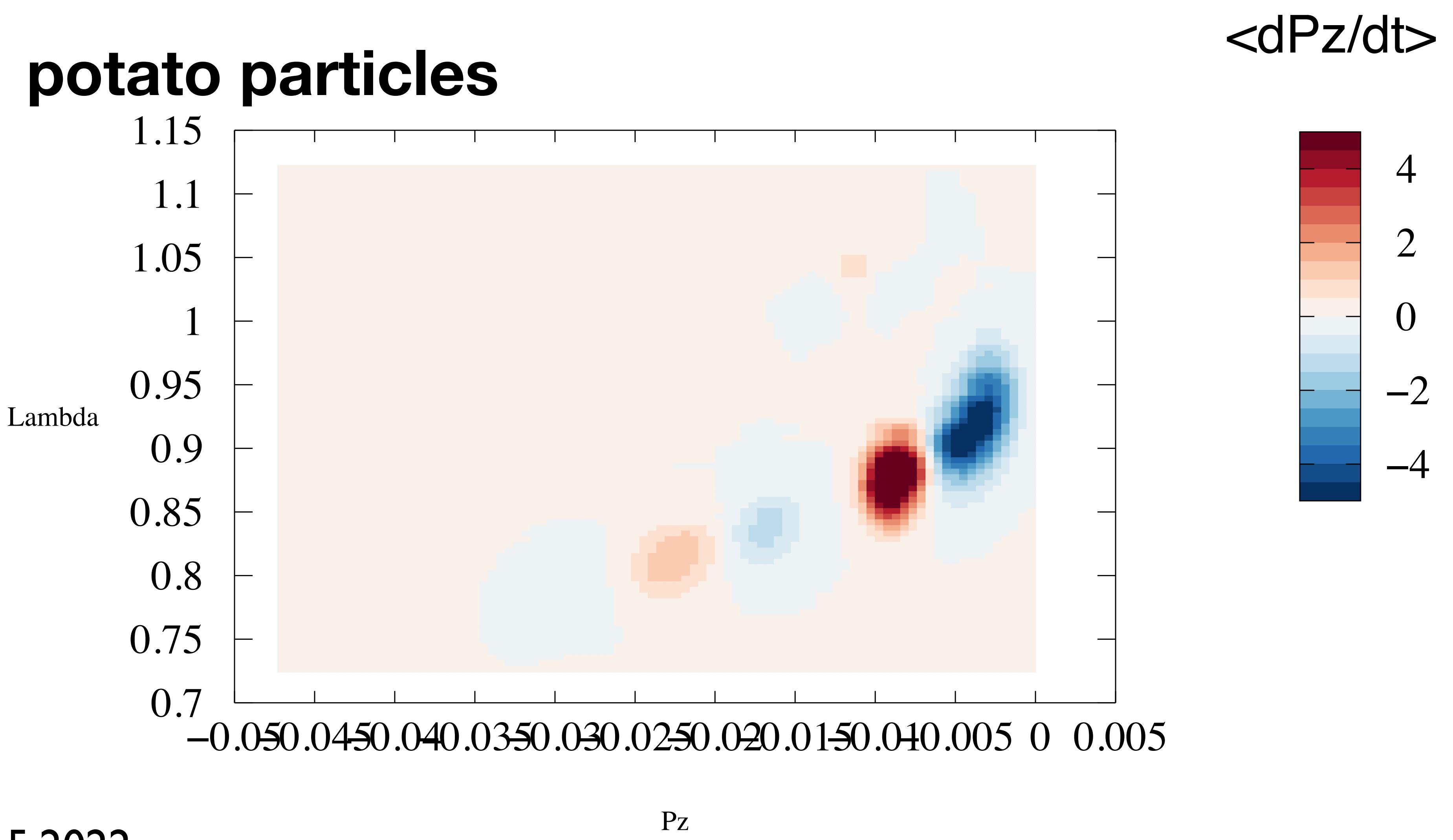
counter-passing particles



trapped particles



potato particles



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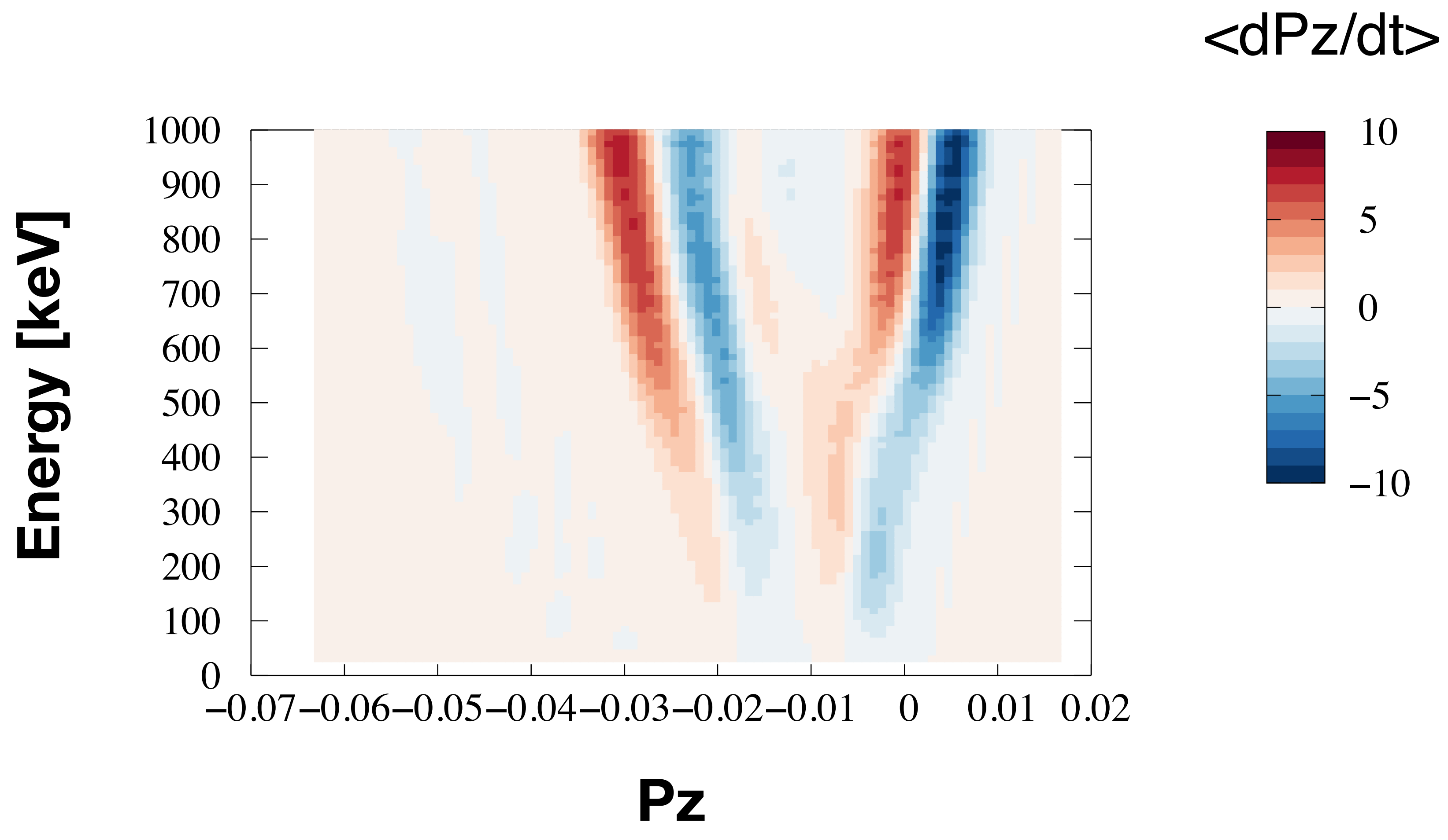
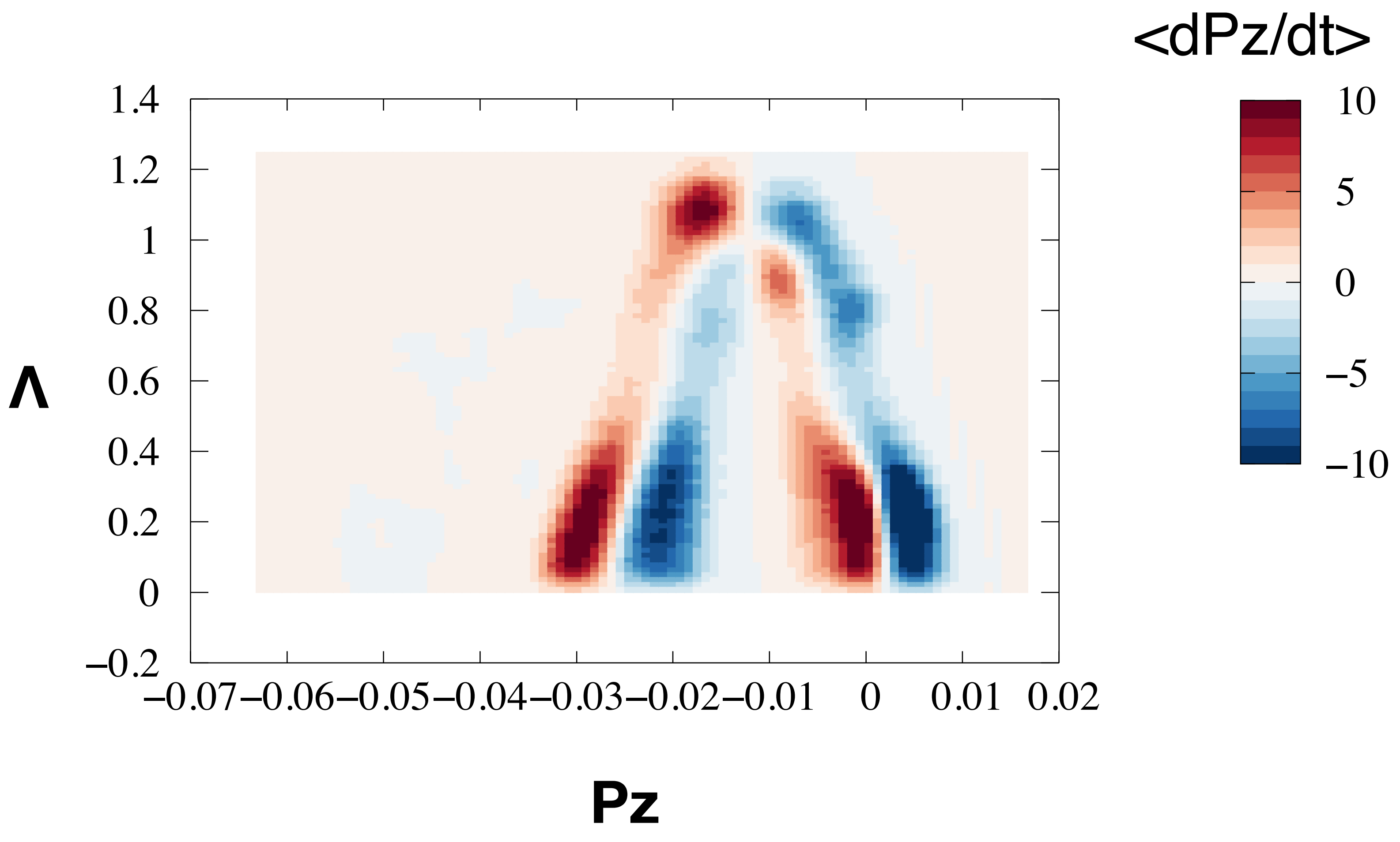
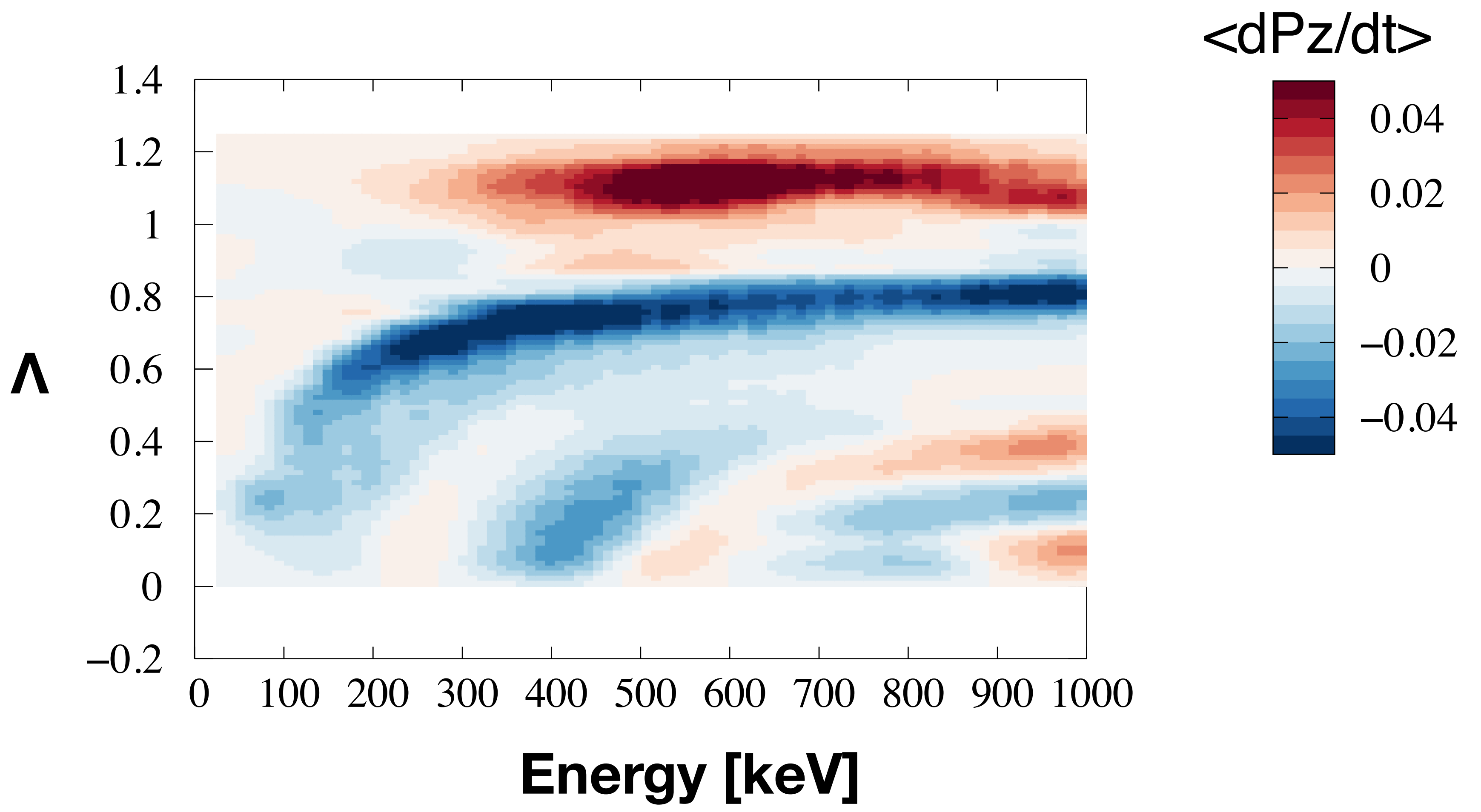
all particles:

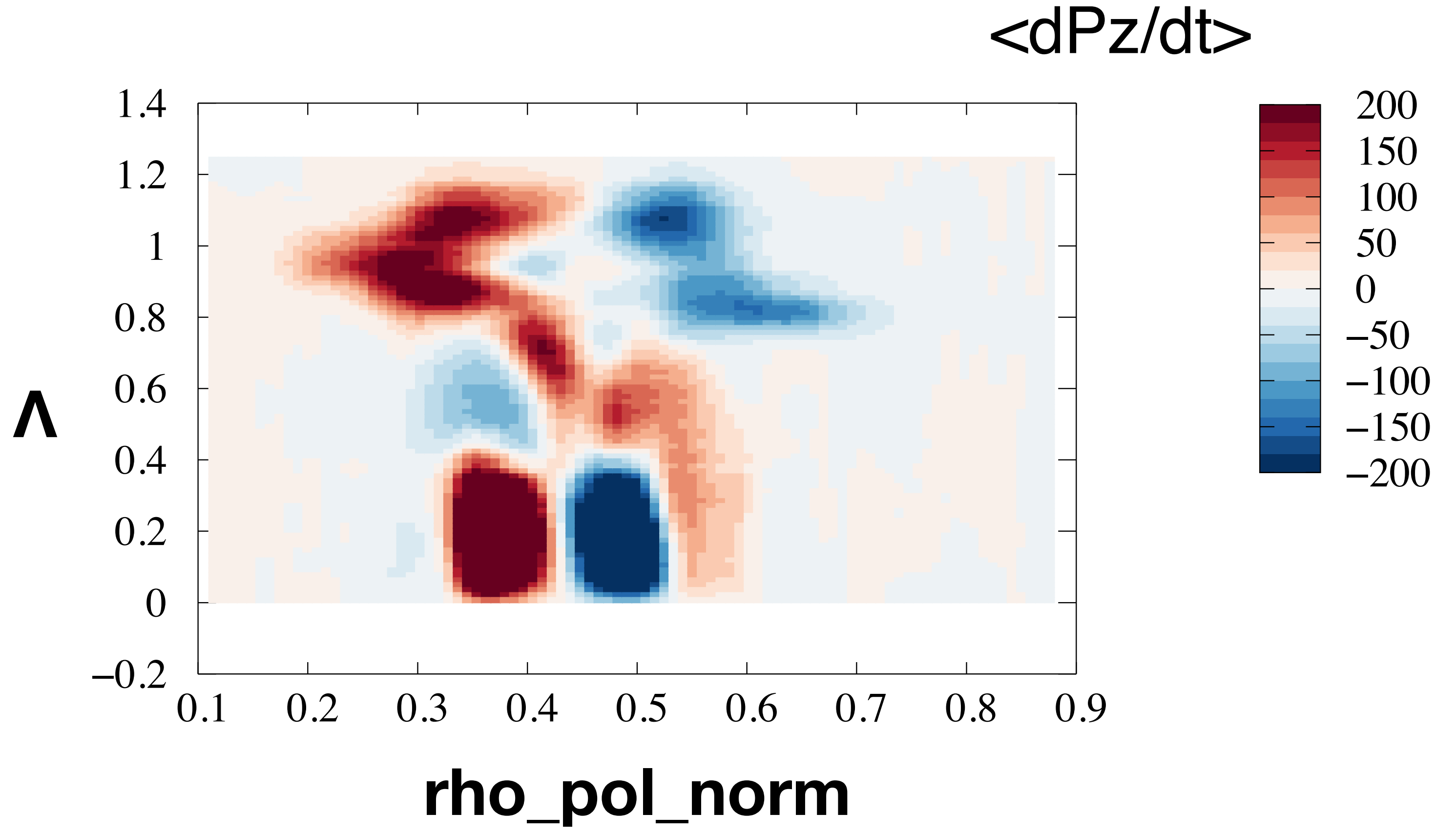


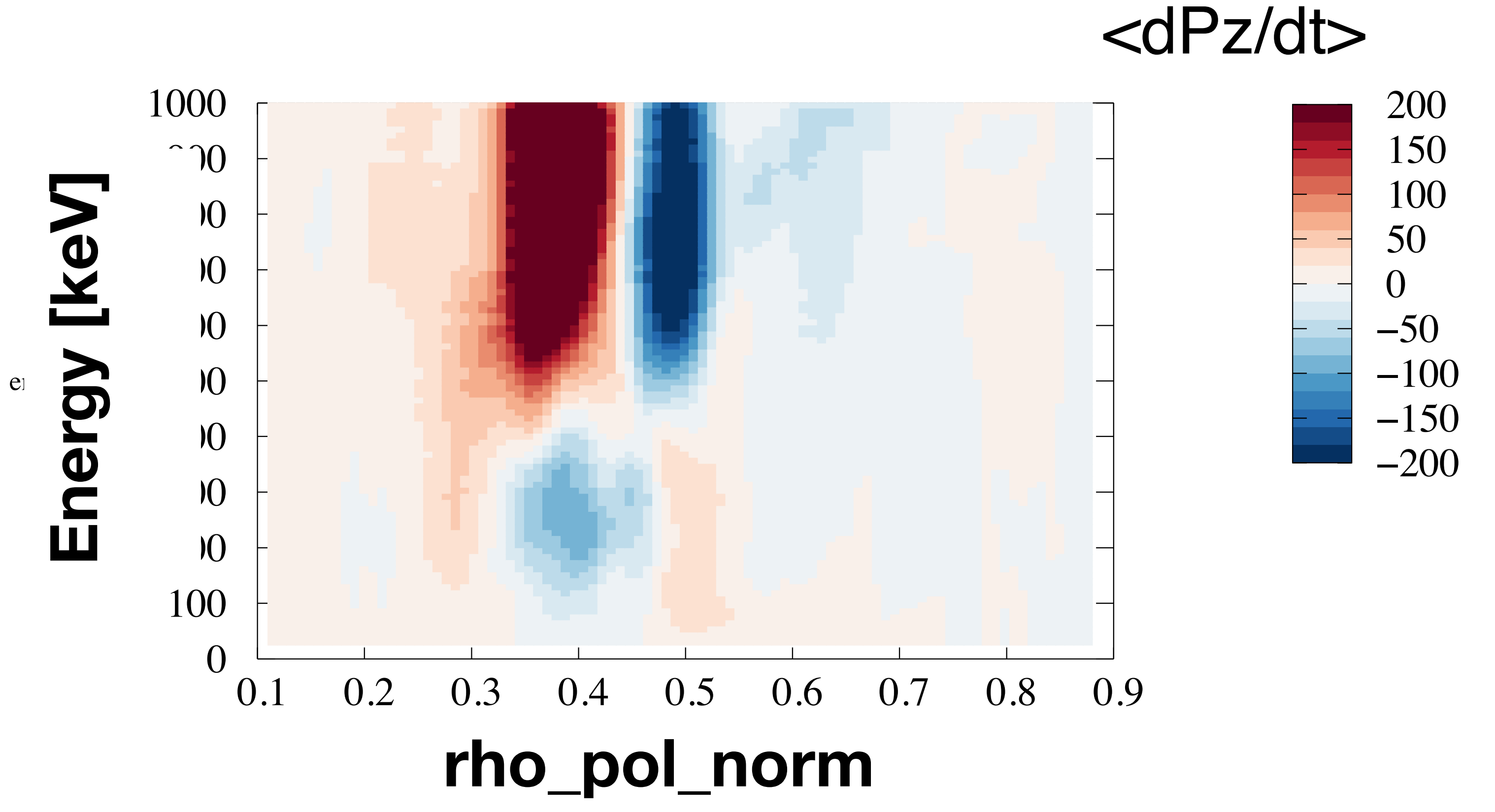




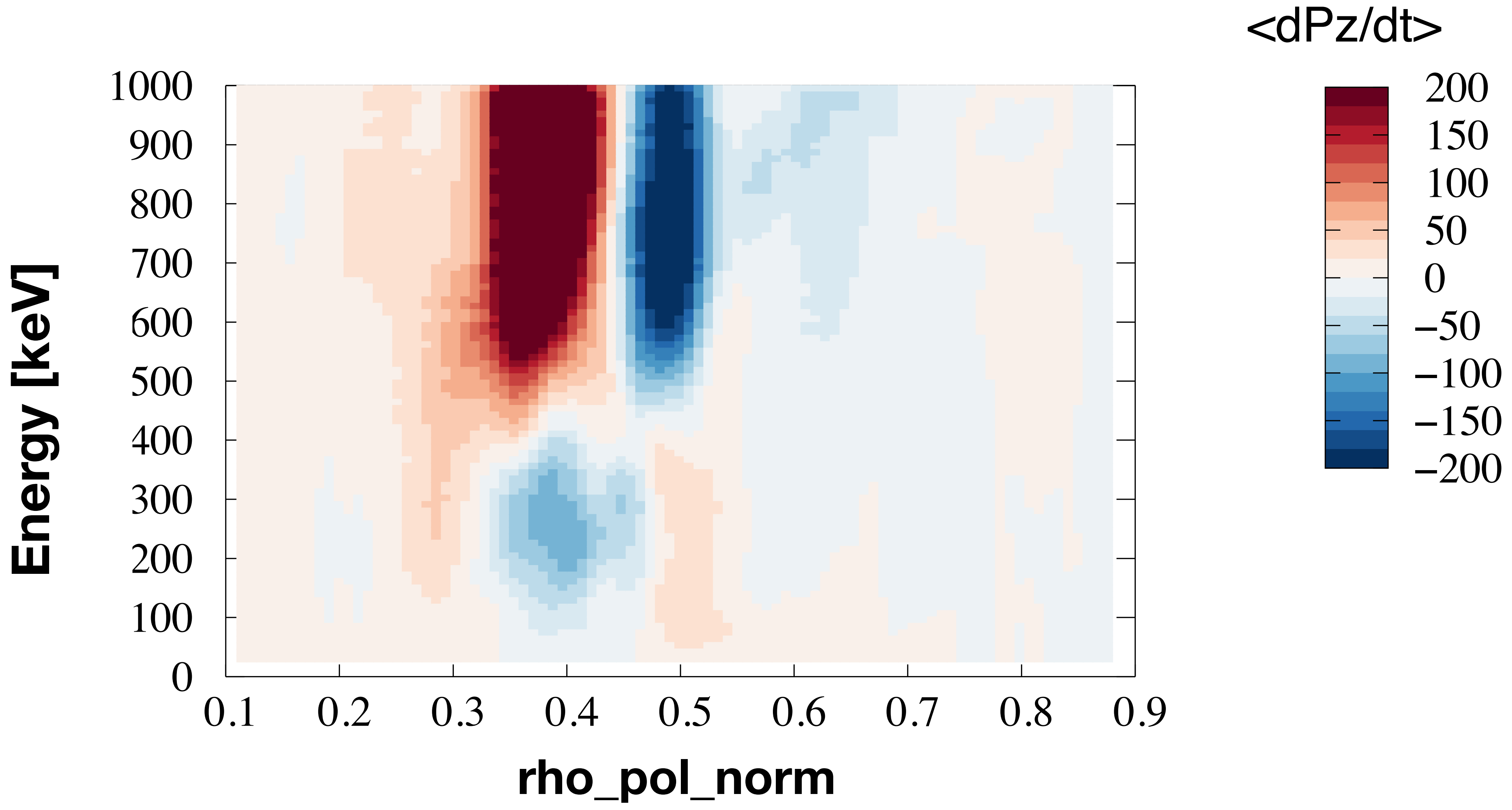
can be easily mapped to <s>:

similar for dE/dt

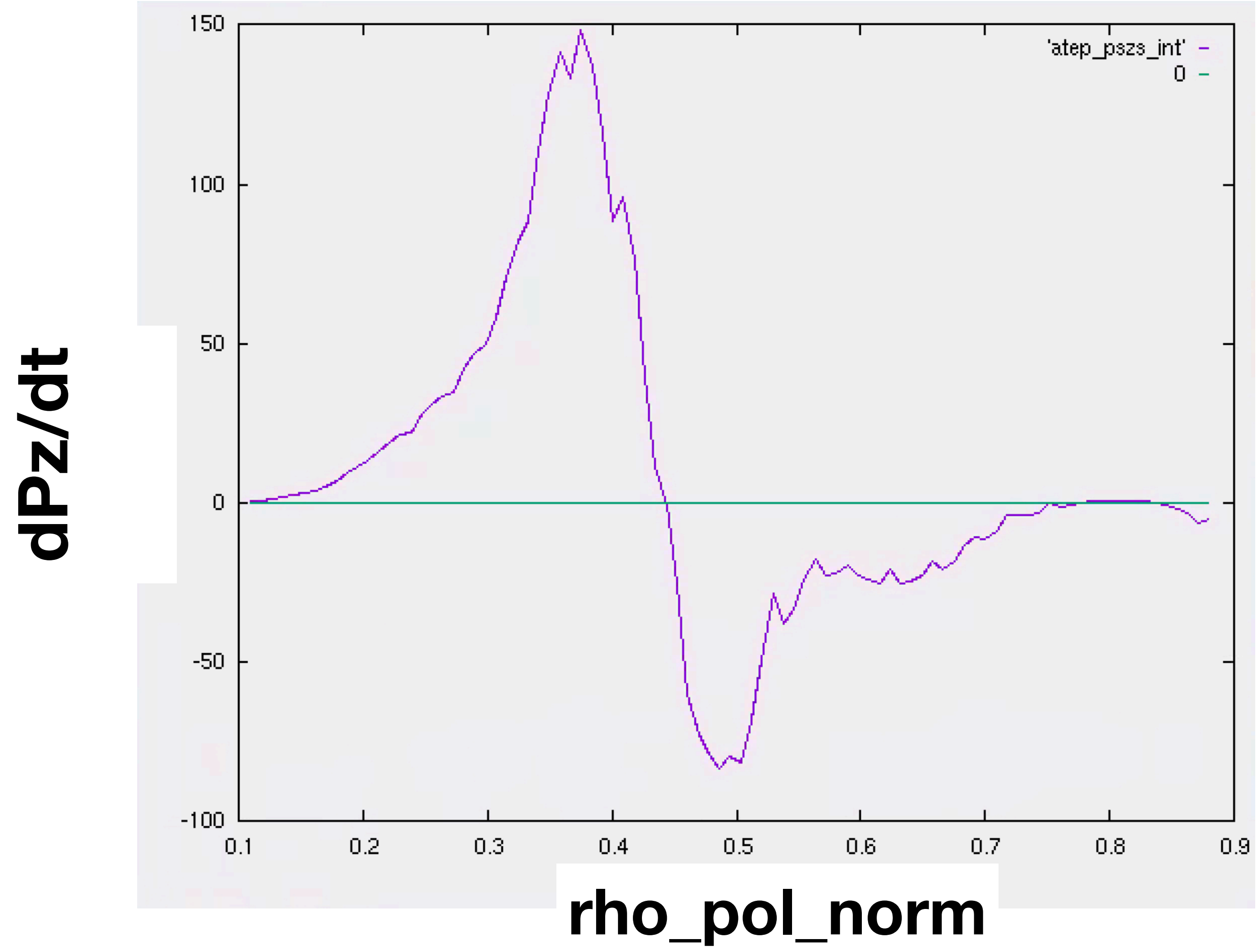




diffusions coefficients: D(s,E) and D(s)

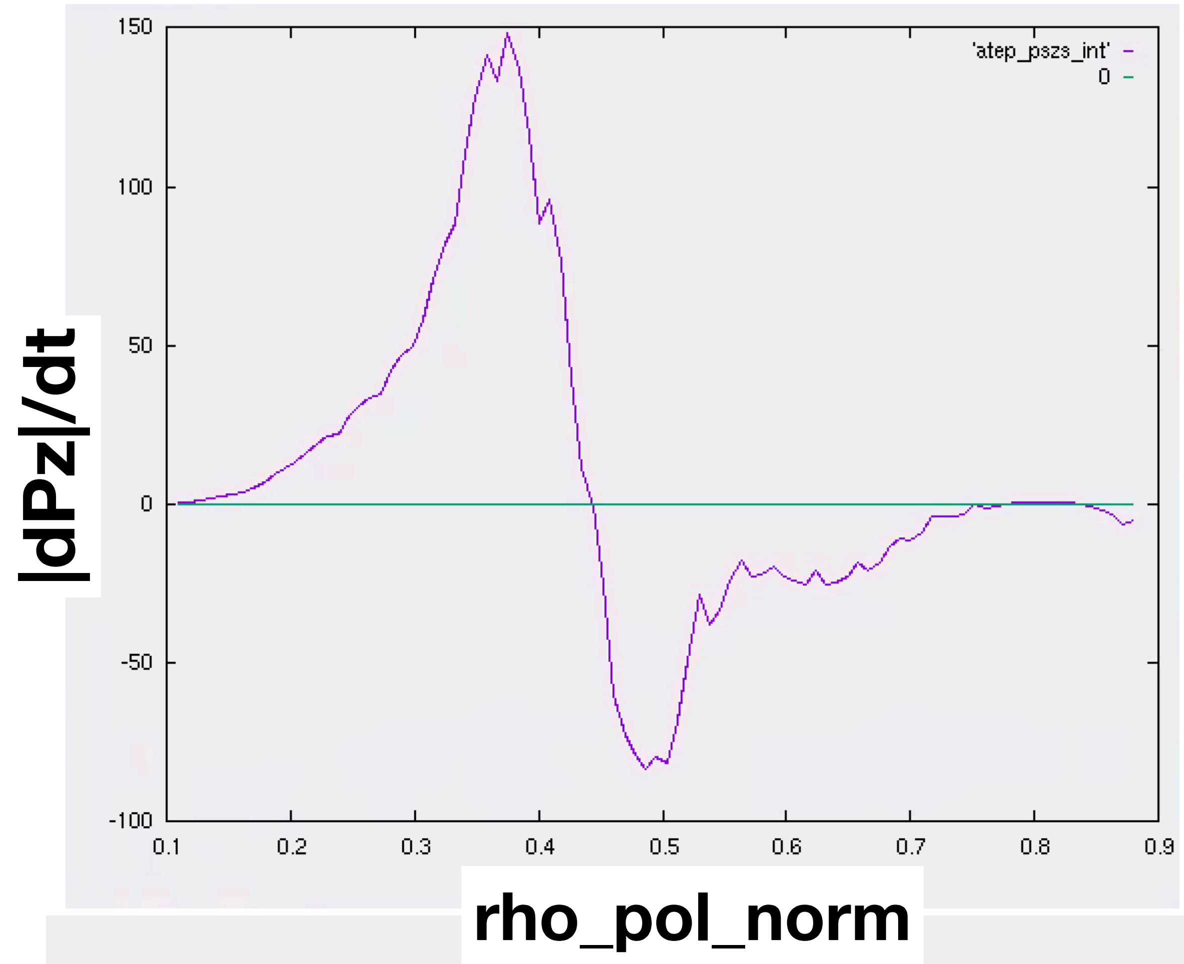


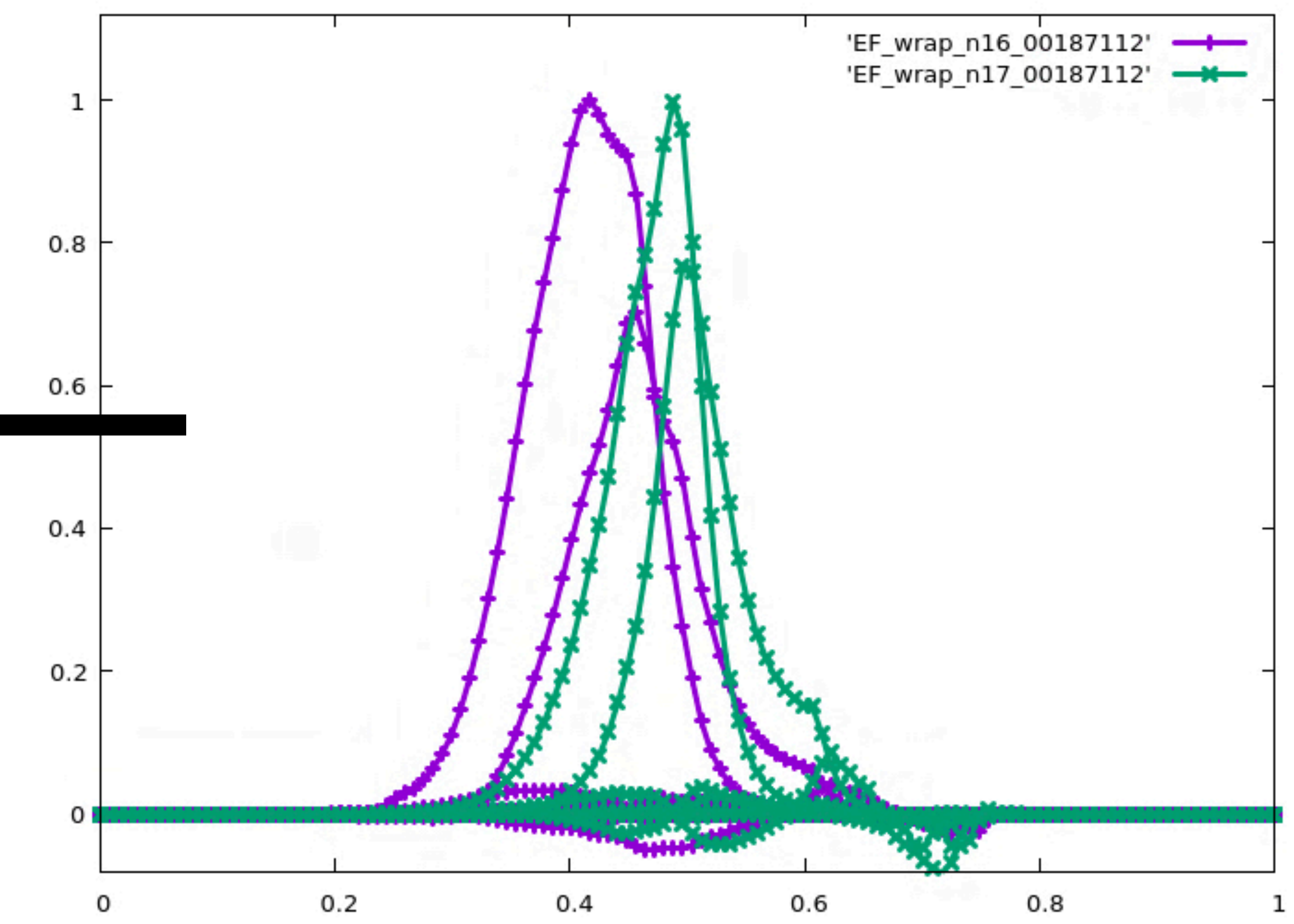
E integration →

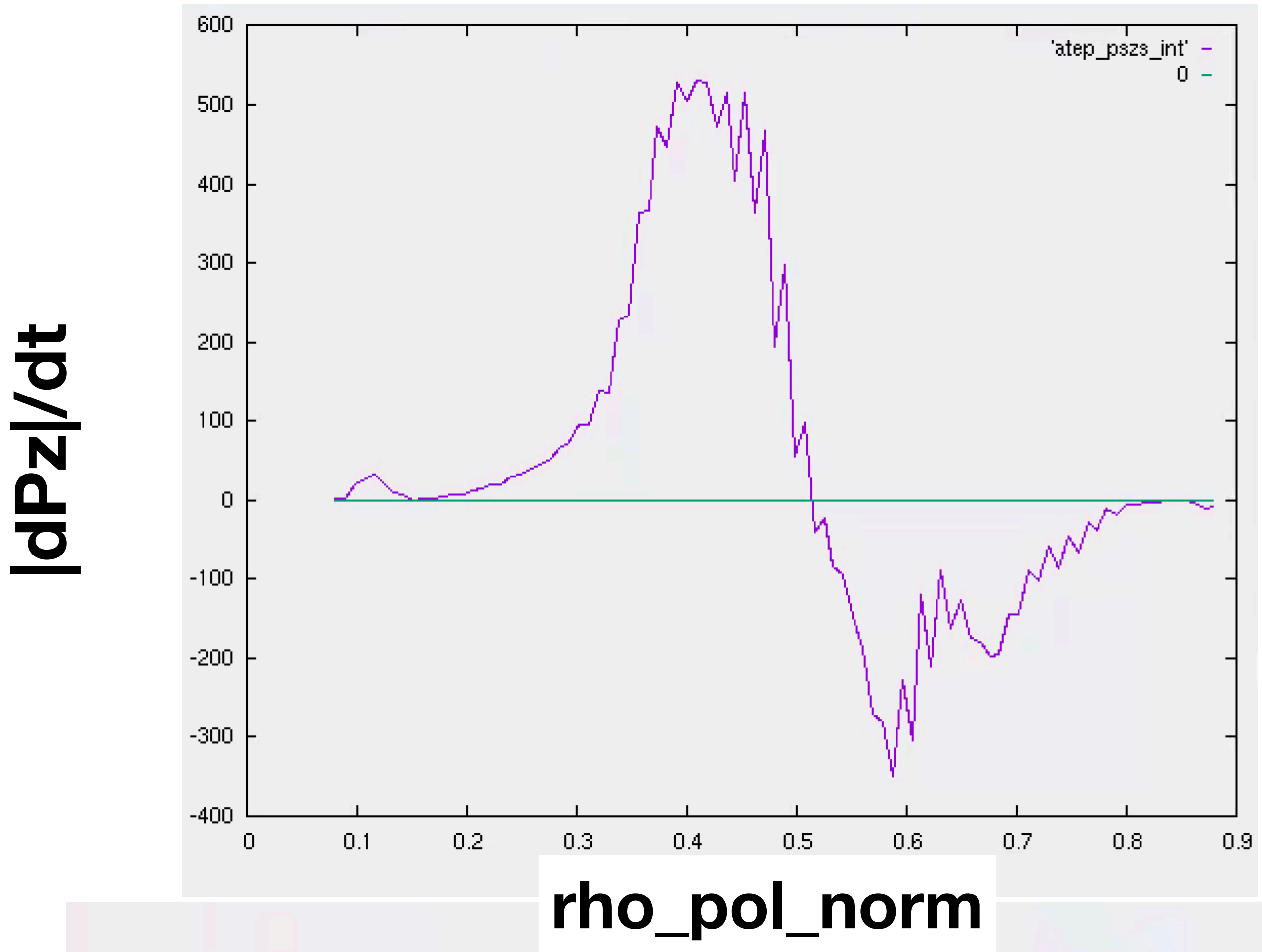


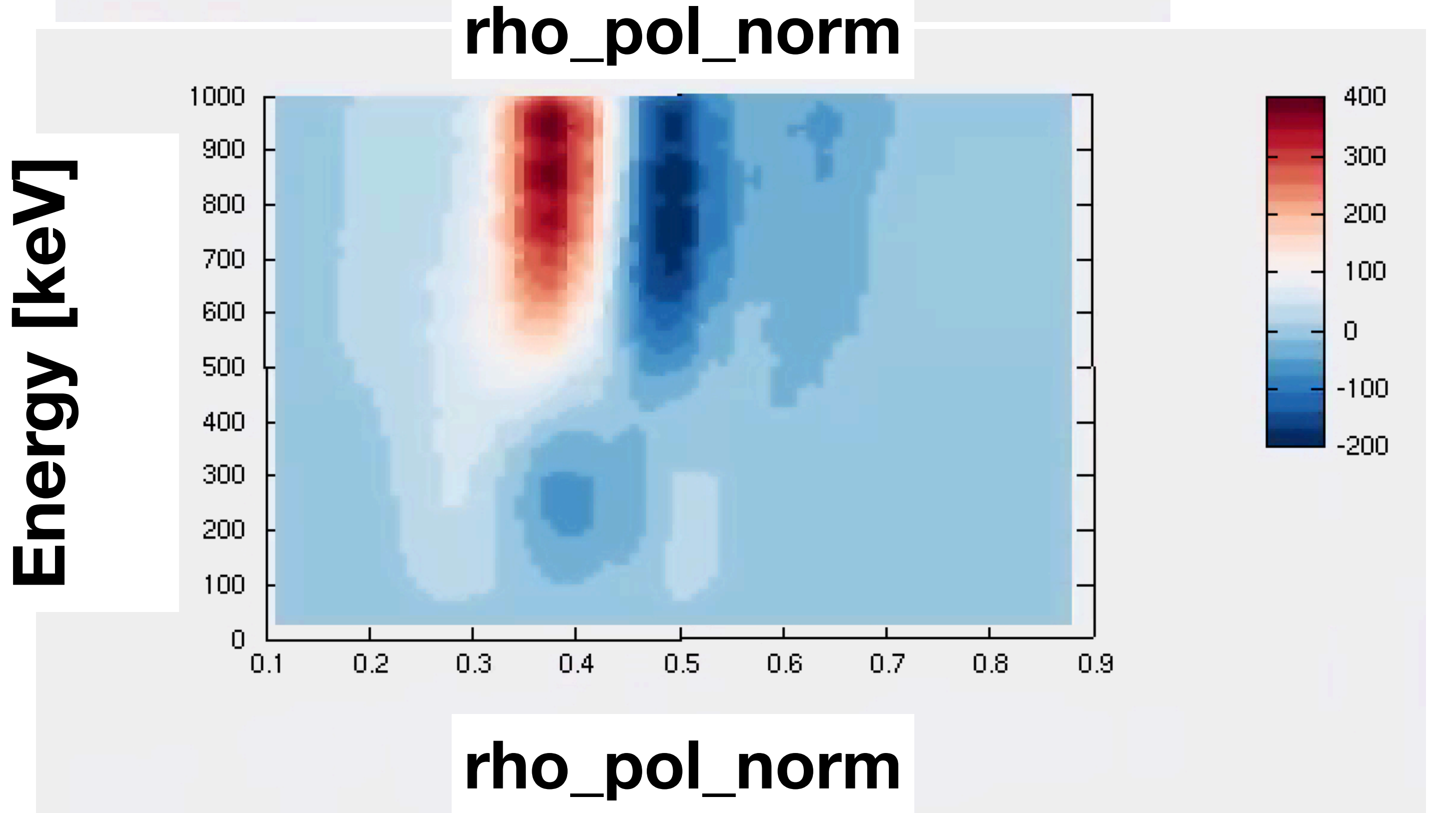
to be done: transform into $D(s,E)=\langle s\rangle^2/\langle t\rangle$
and feed back to transport code

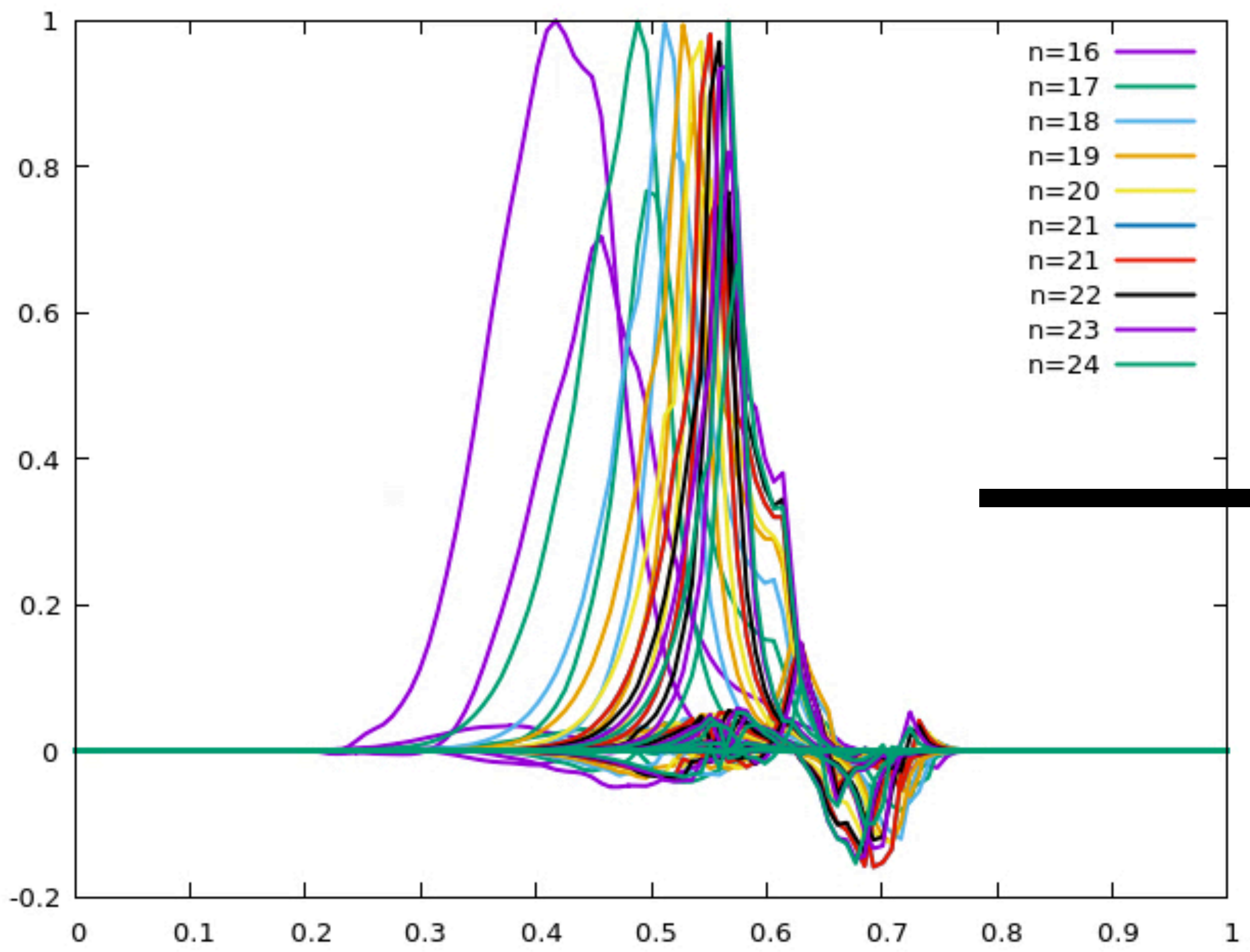
broadened spectrum of modes: n=16-24, all with fixed amplitude (dB/B=5*10⁻³)

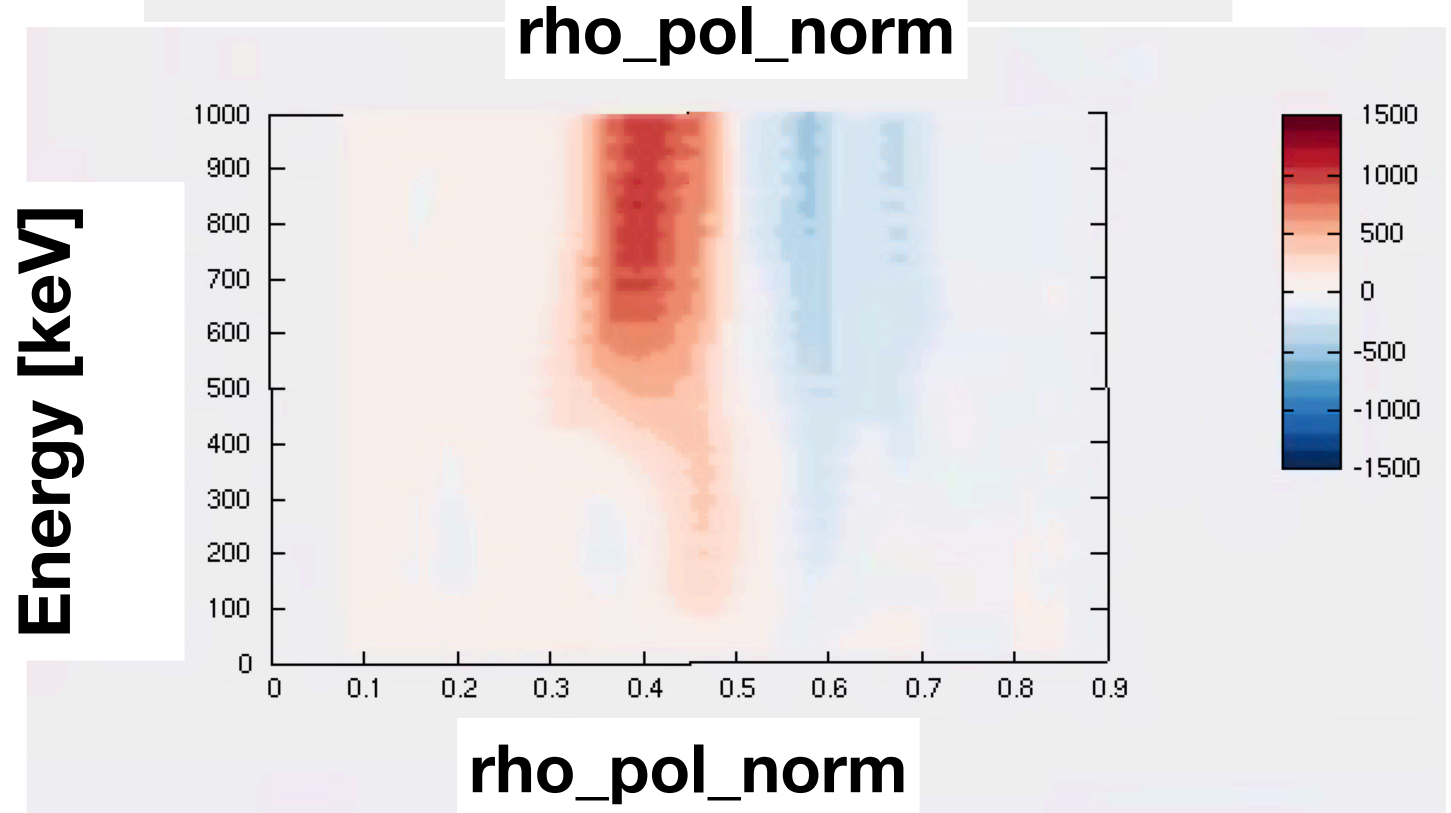


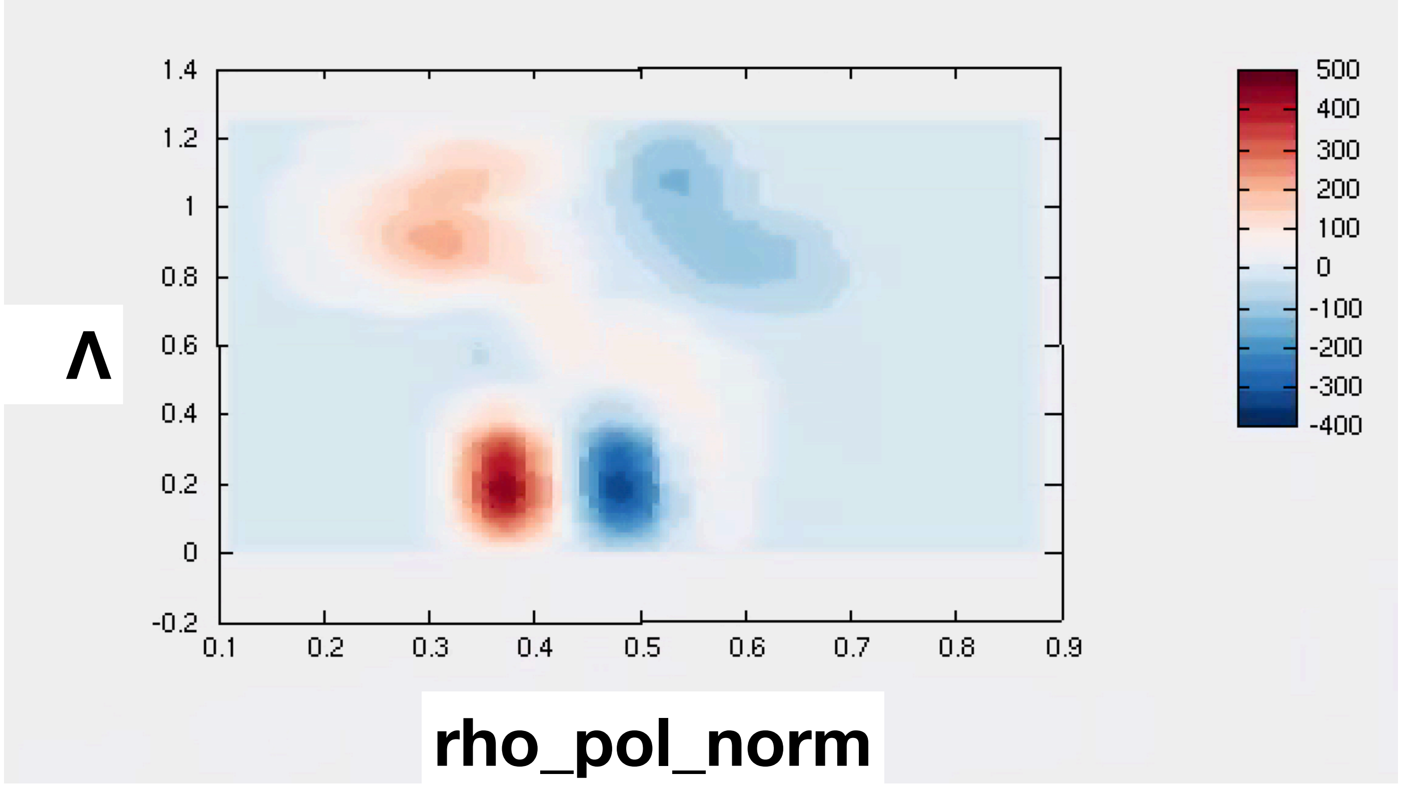


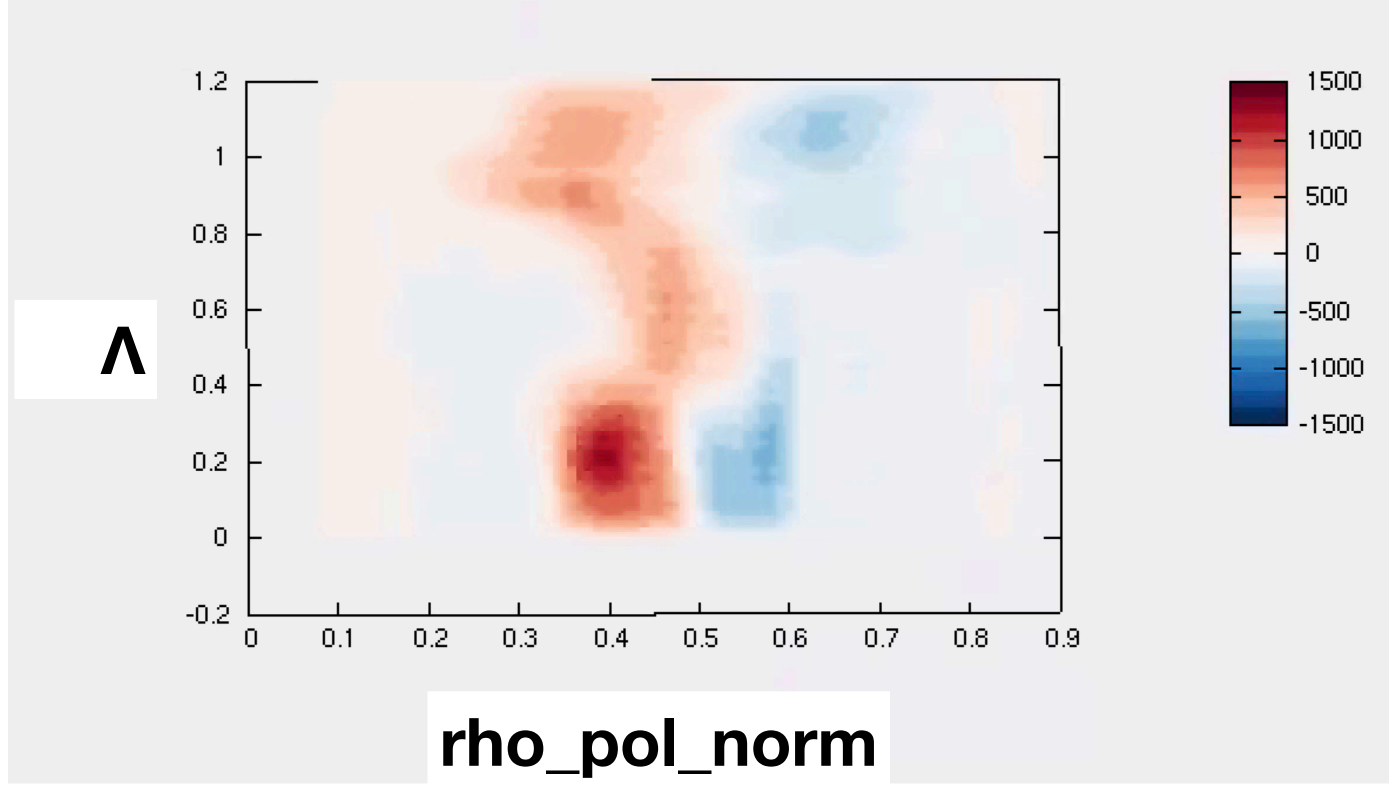






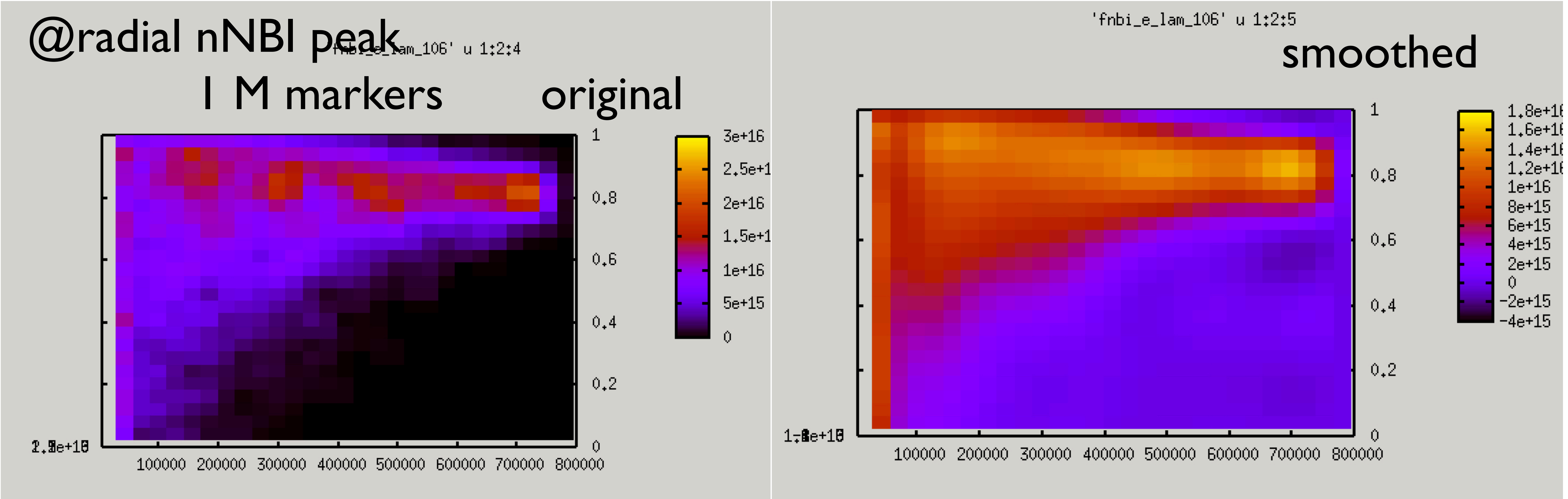


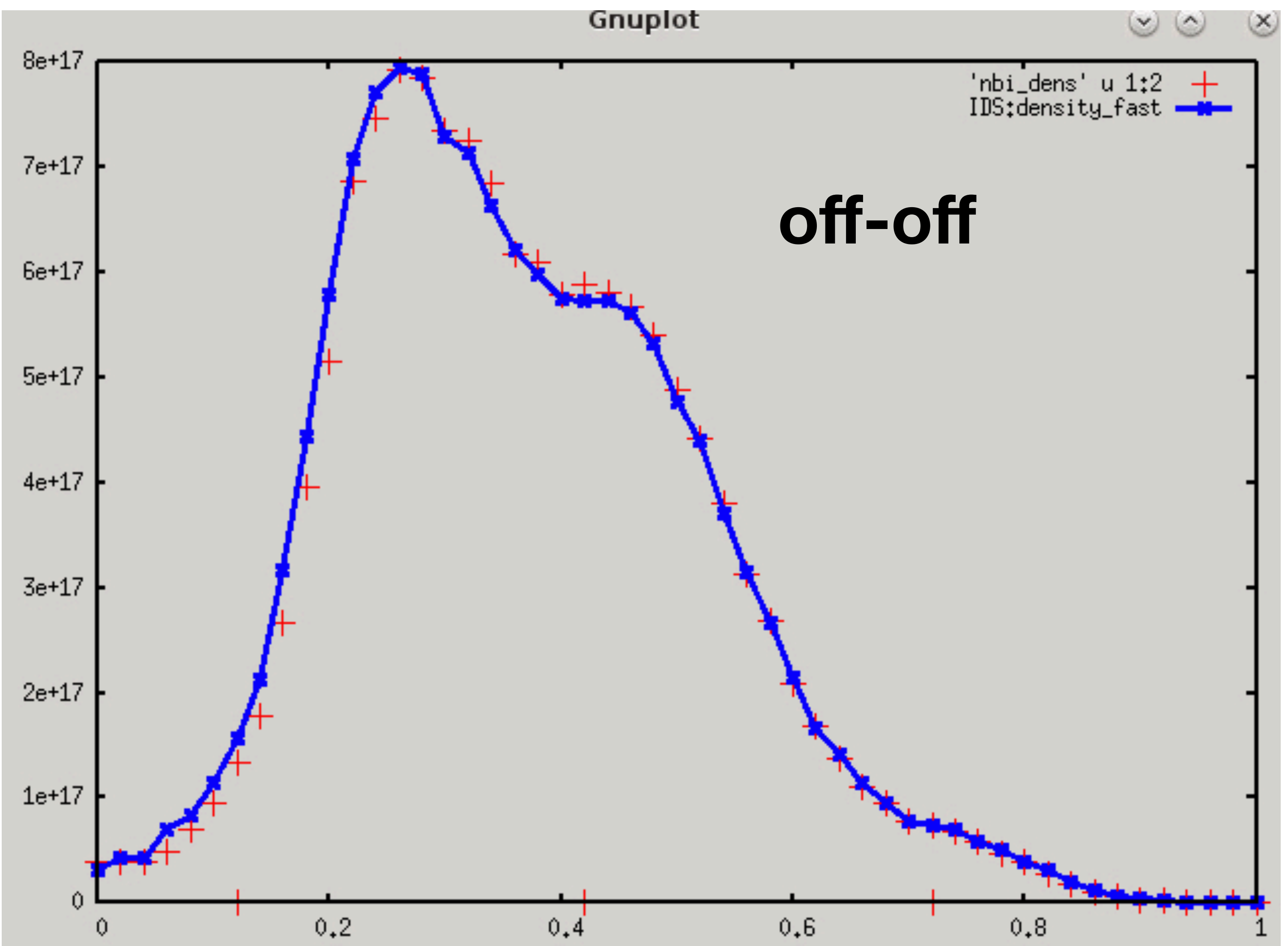


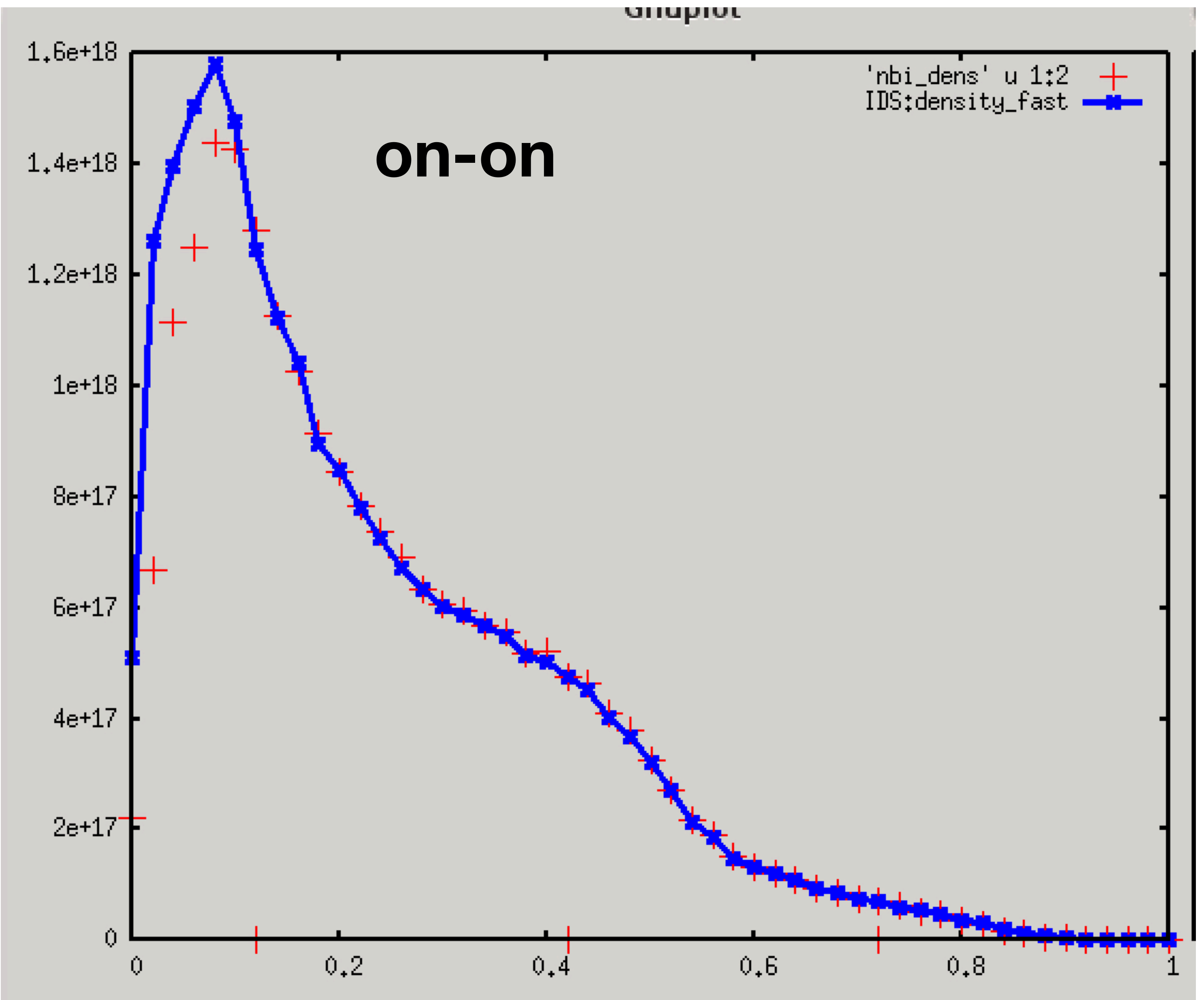


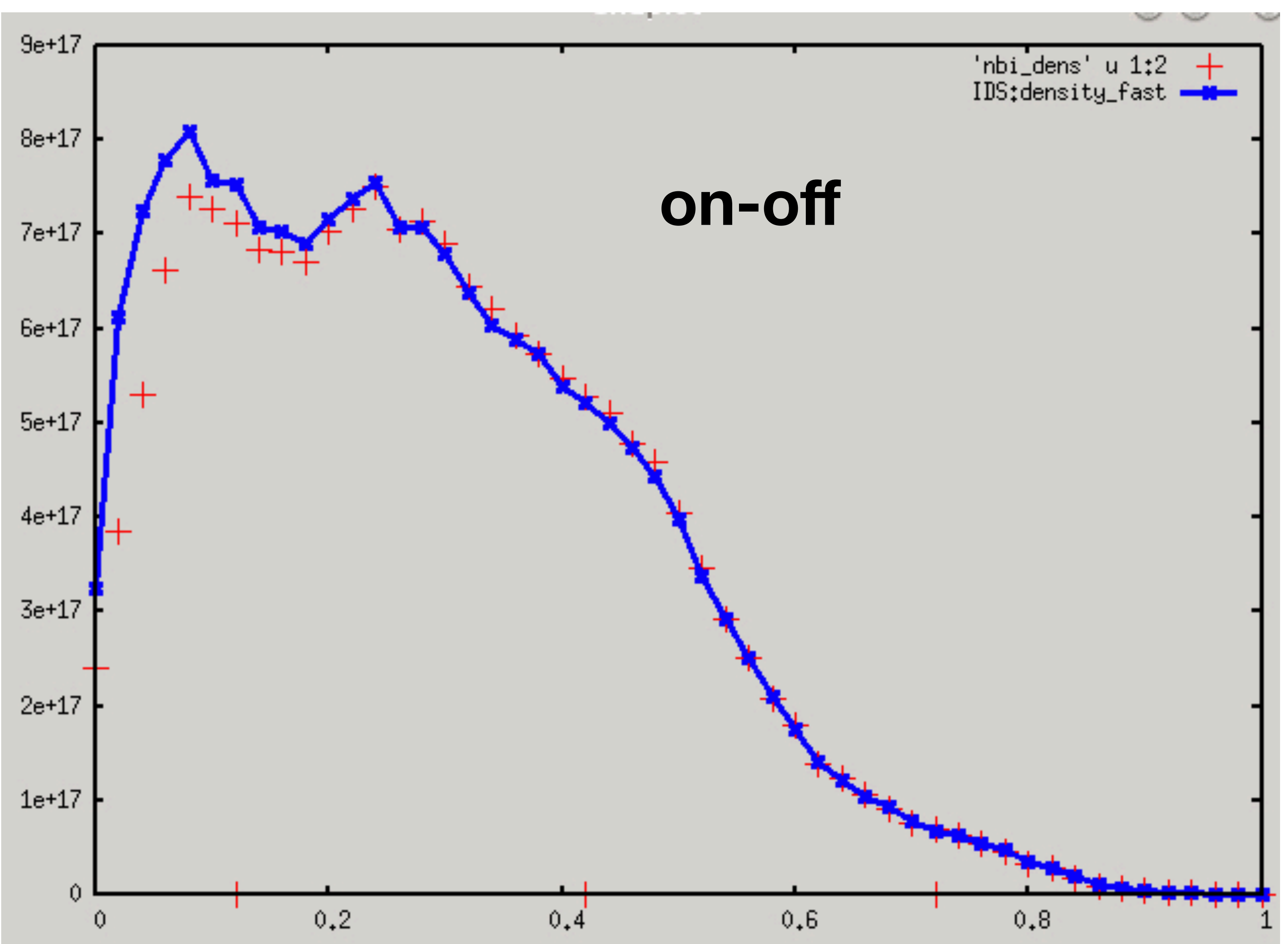
progress on implementation of transport model:
ATEP code

ITER: 100015: F_{EP} is available from H&CD WF [thx. M. Schneider]



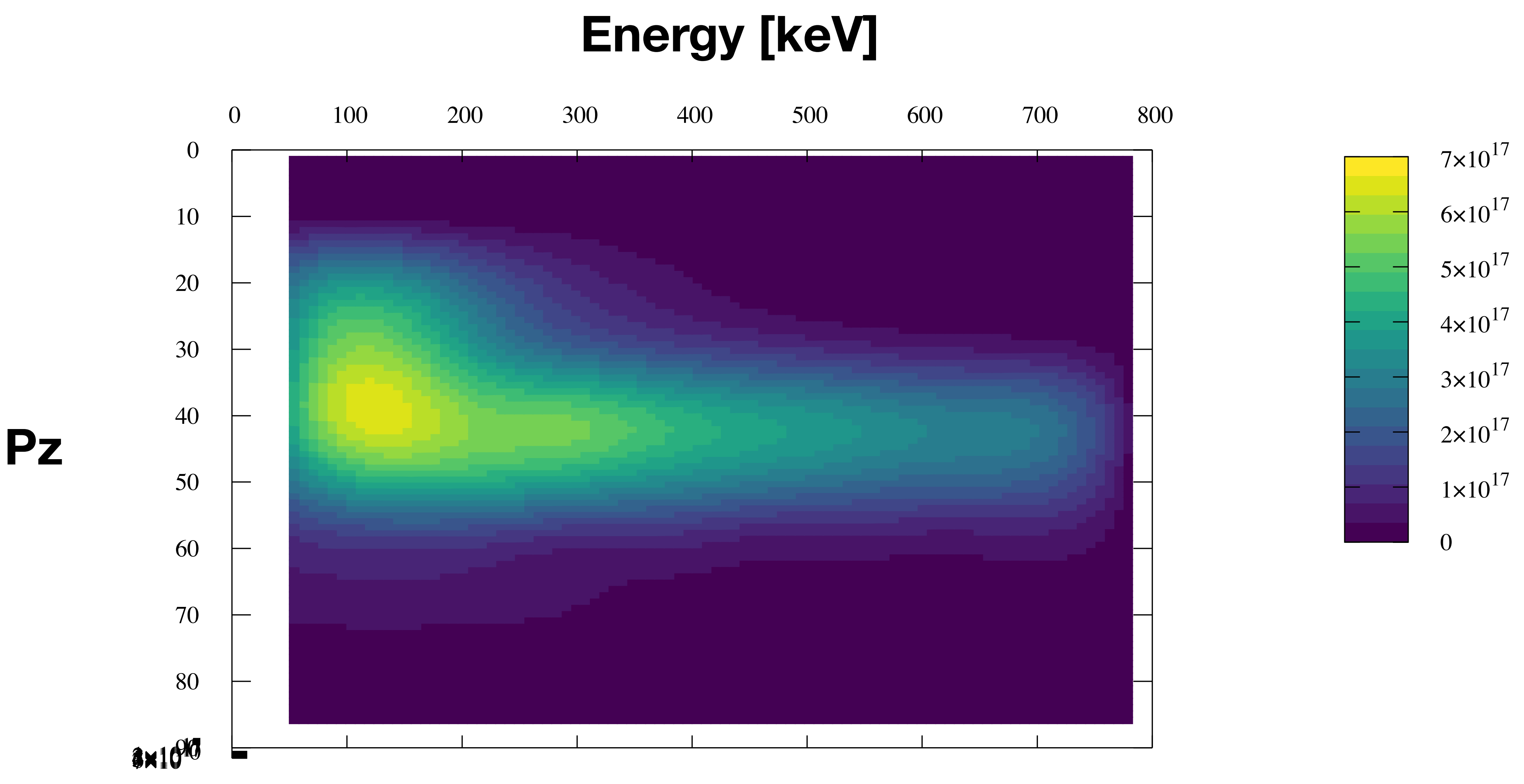


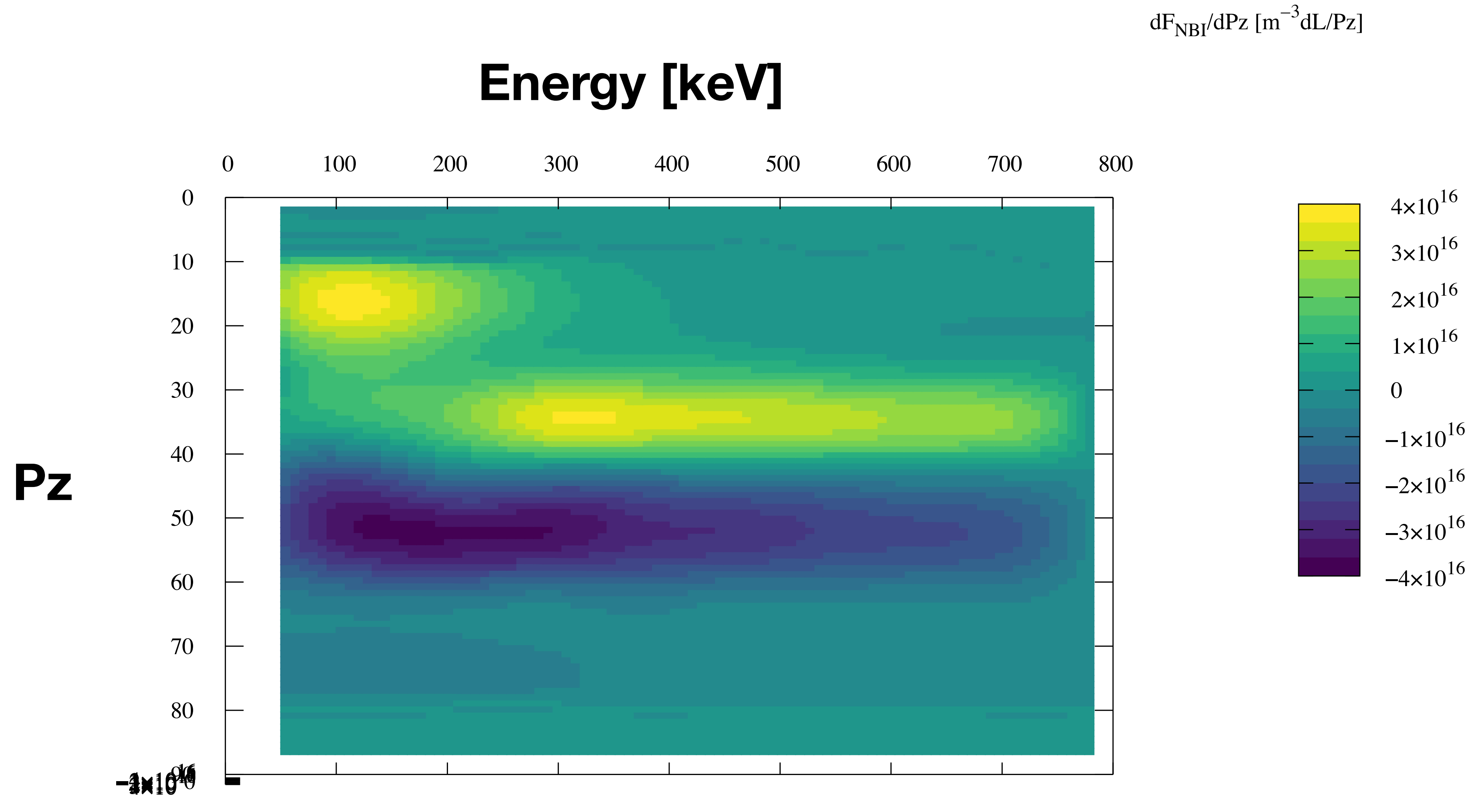


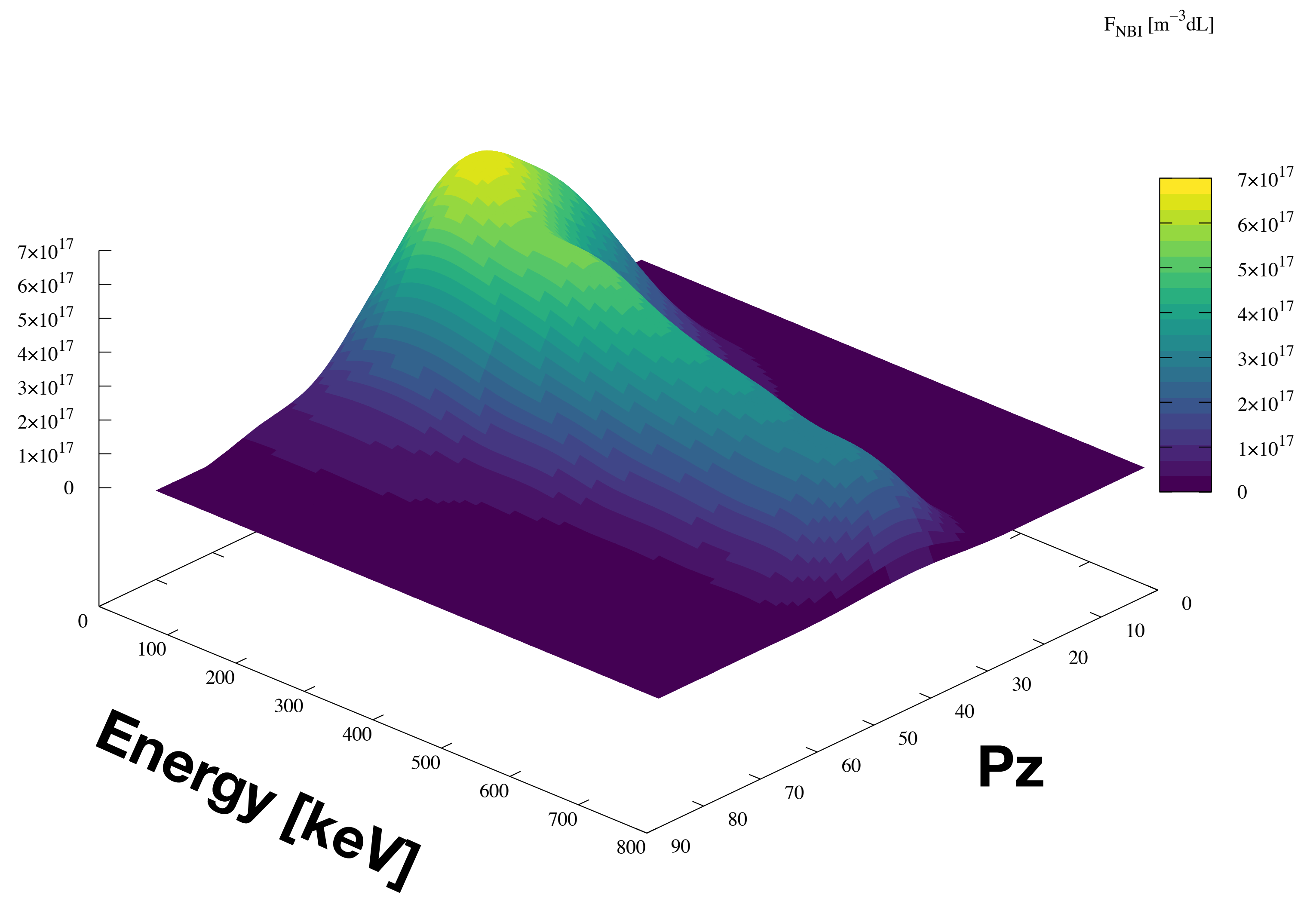


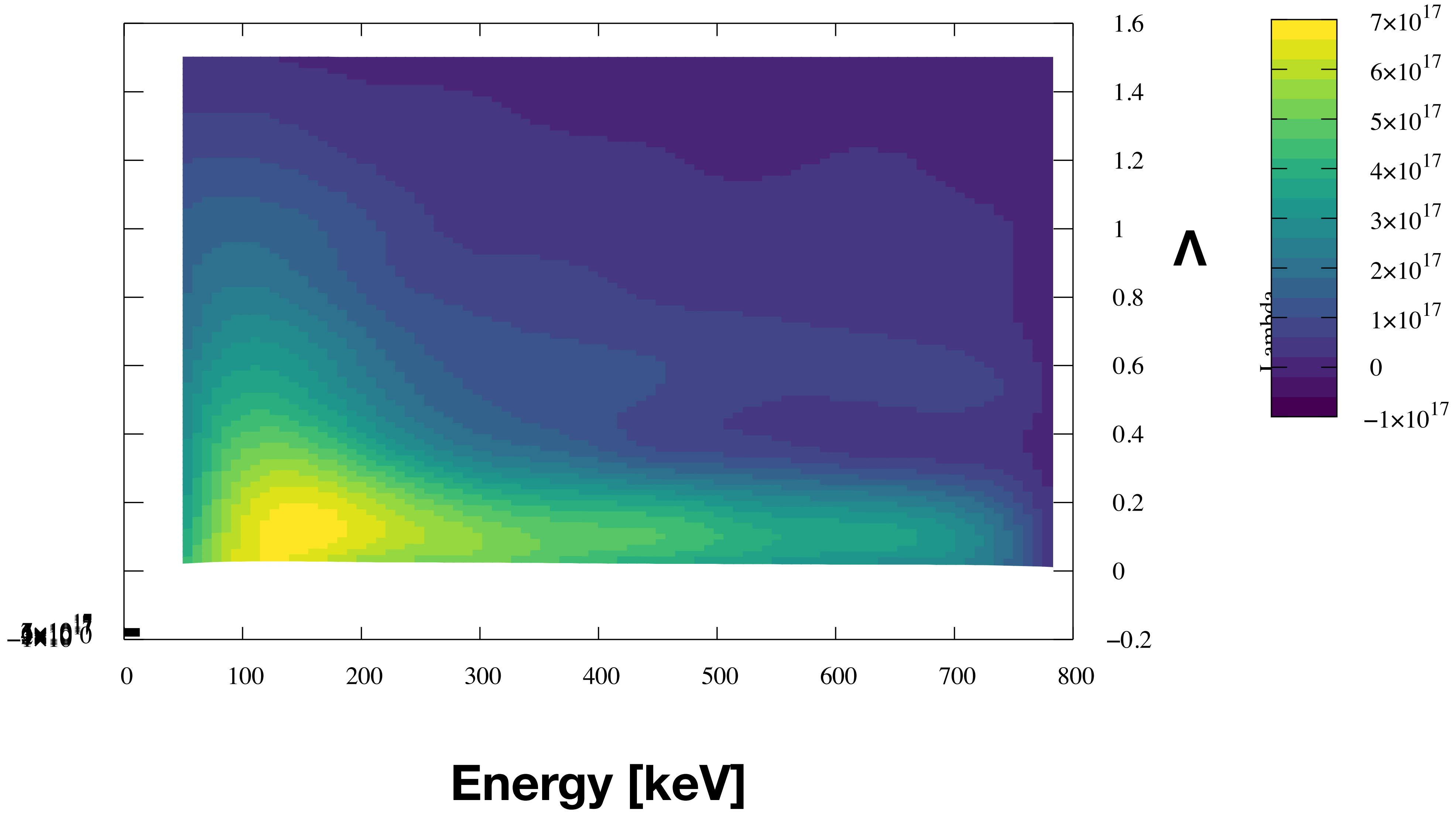
bin/smooth/map to same COM grid as PSZS

binning 1 M markers from H&CD, use 2d bsplines with smoothing in (Pz,E), (Pz,Λ) and (E,Λ), construct 3d spline









ATEP code: advance transport equation

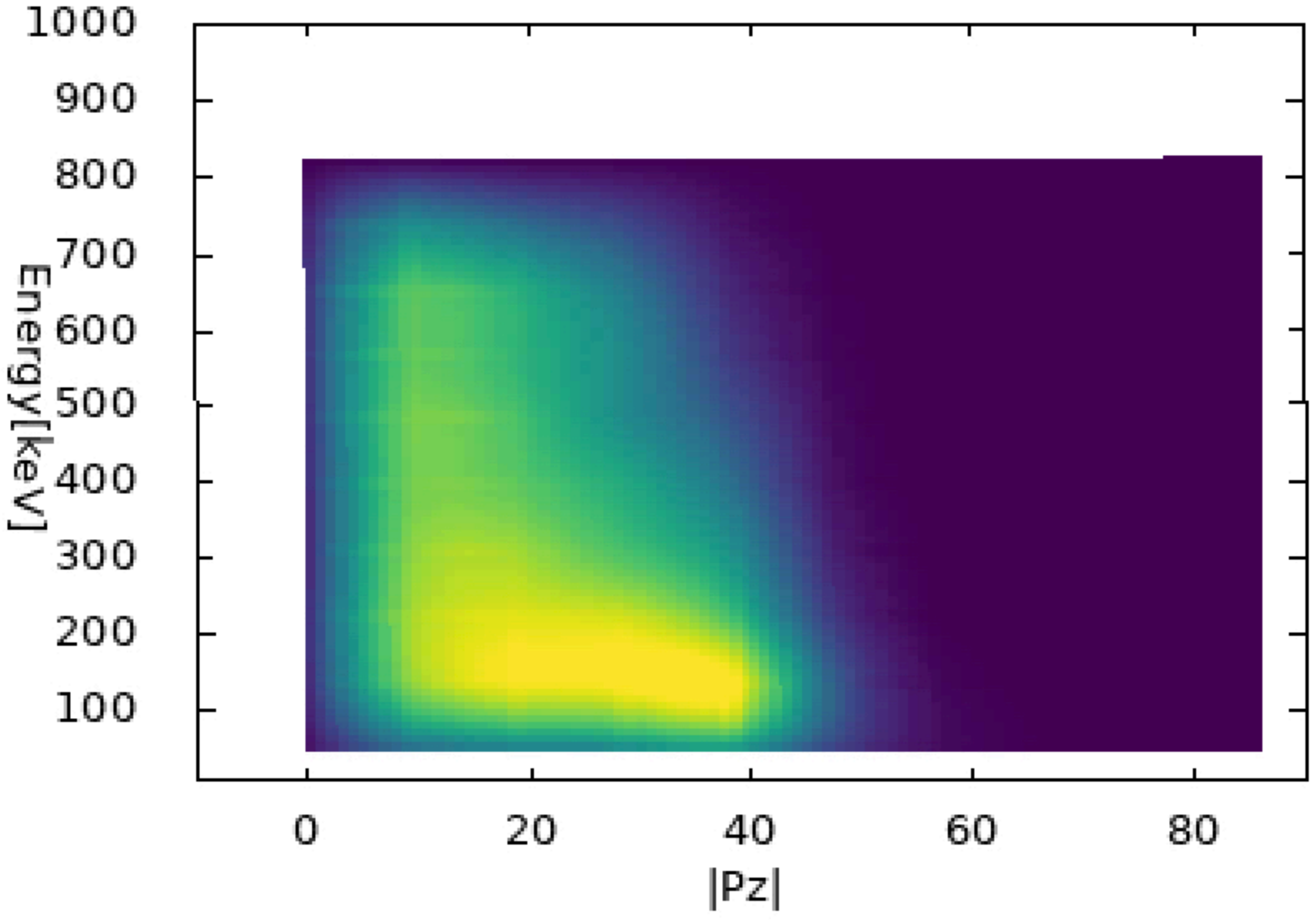
simple finite difference scheme to start with (final scheme to be decided when sources/collisions are implemented):

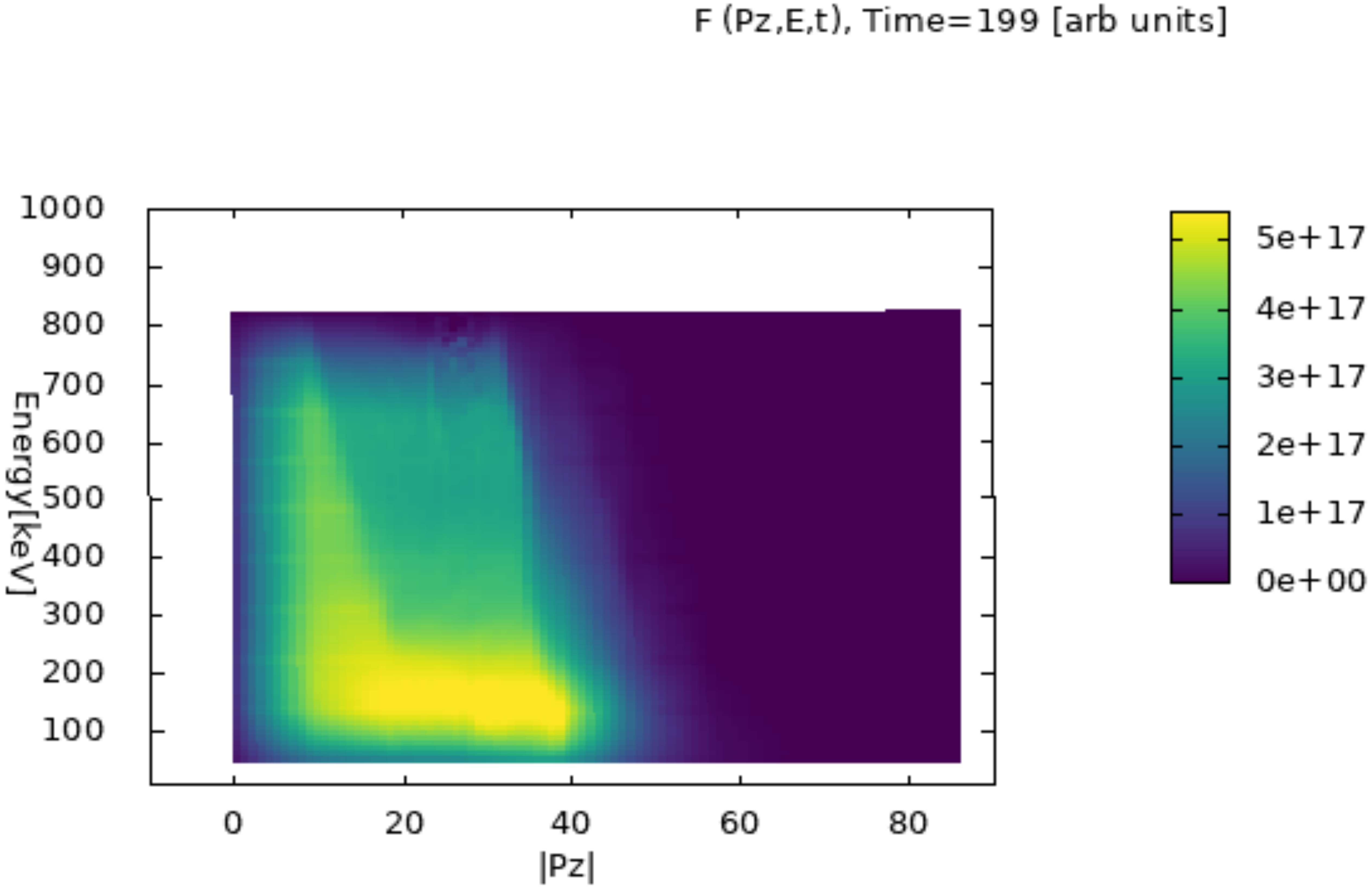
$$\frac{\partial F_{EP}}{\partial t} = \frac{\partial Pz}{\partial t}\frac{\partial F_{EP}}{\partial P_z} + \frac{\partial E}{\partial t}\frac{\partial F_{EP}}{\partial E}$$

note: $\frac{\partial^2 Pz}{\partial t \partial P_z} F_{EP}$ **term excluded so far: dPz/dt assumed constant -> kick model limit**

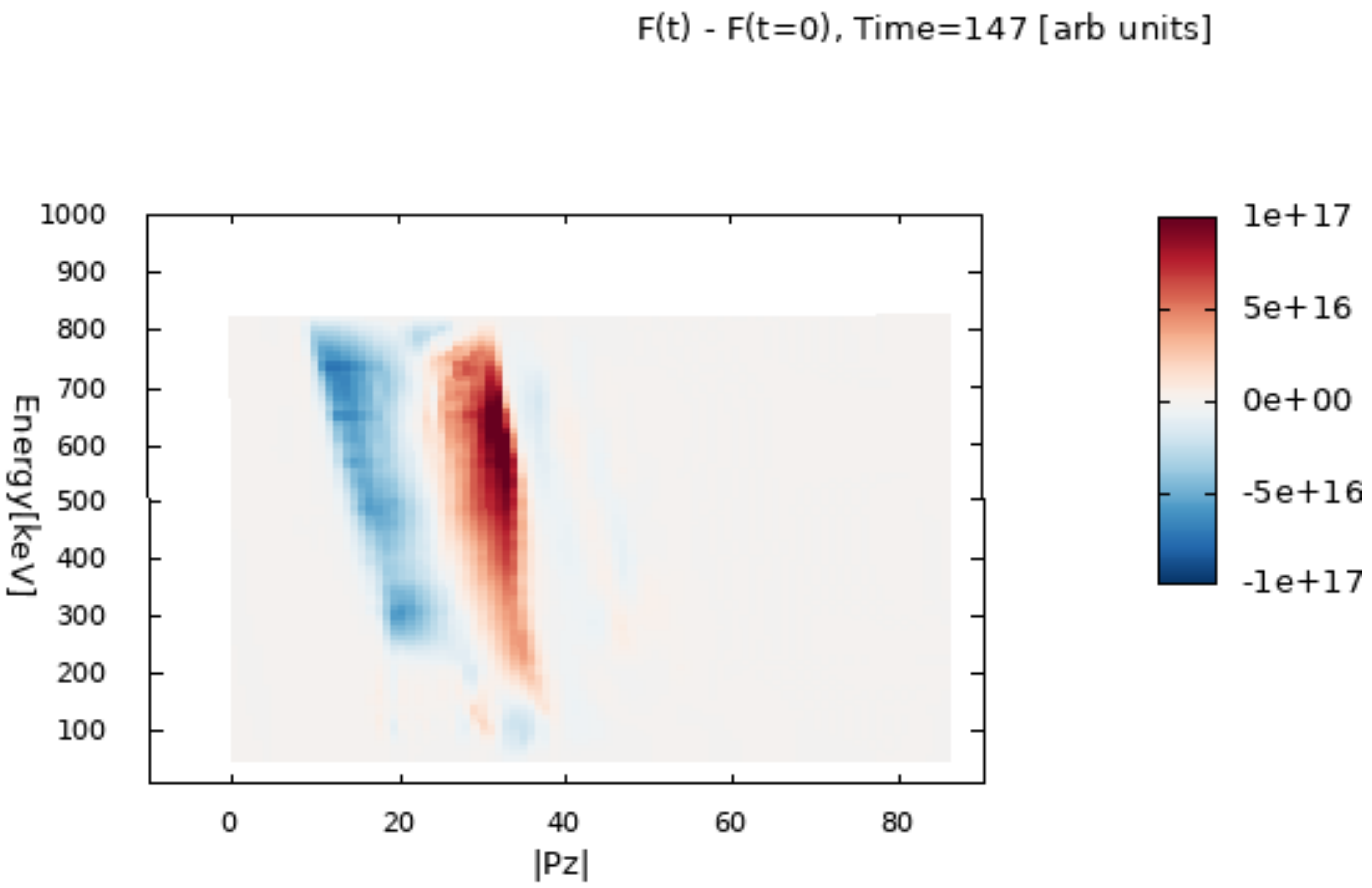
runtime: several seconds

FEP at start:



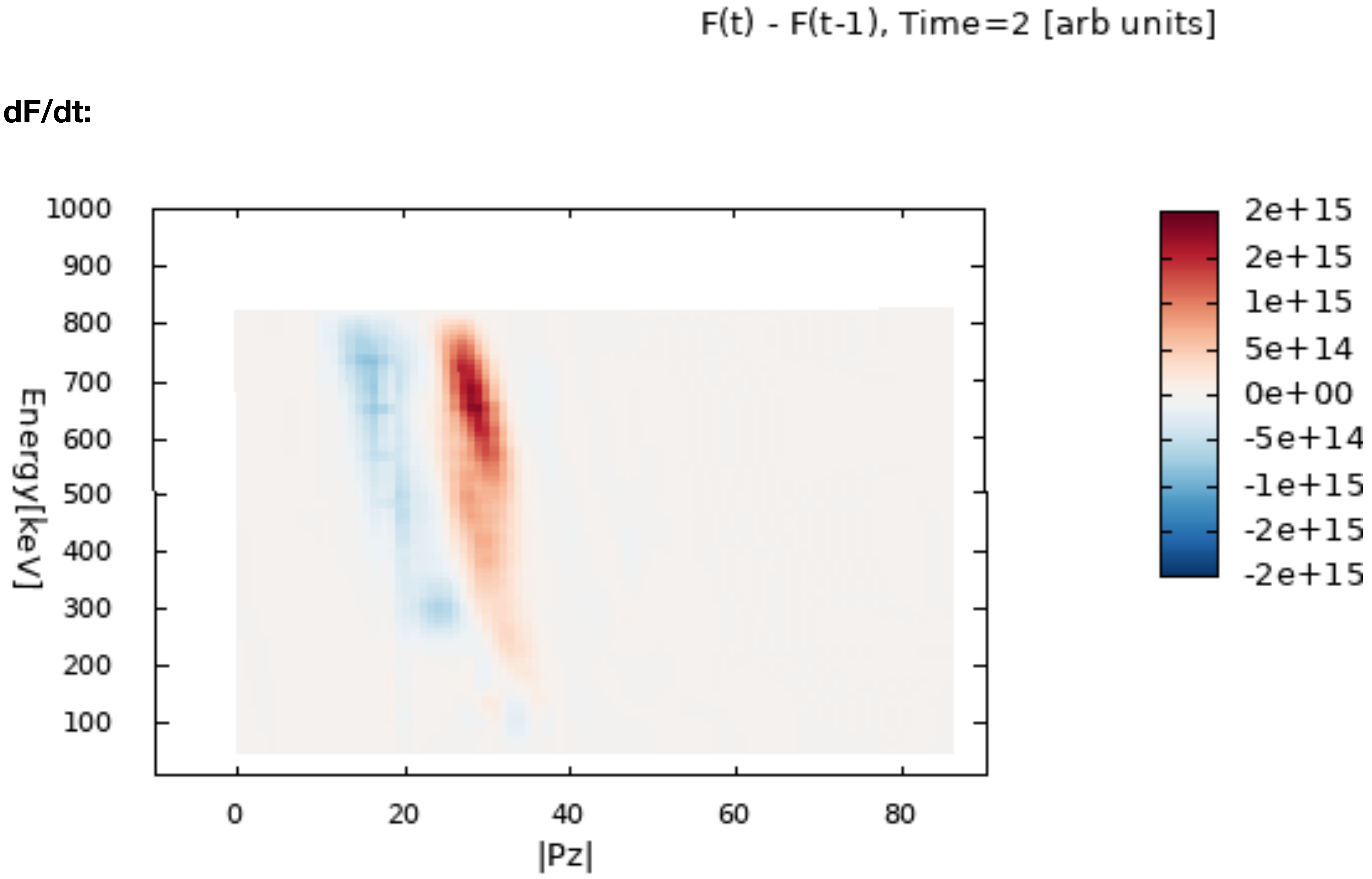


ATEP code: advance transport equation

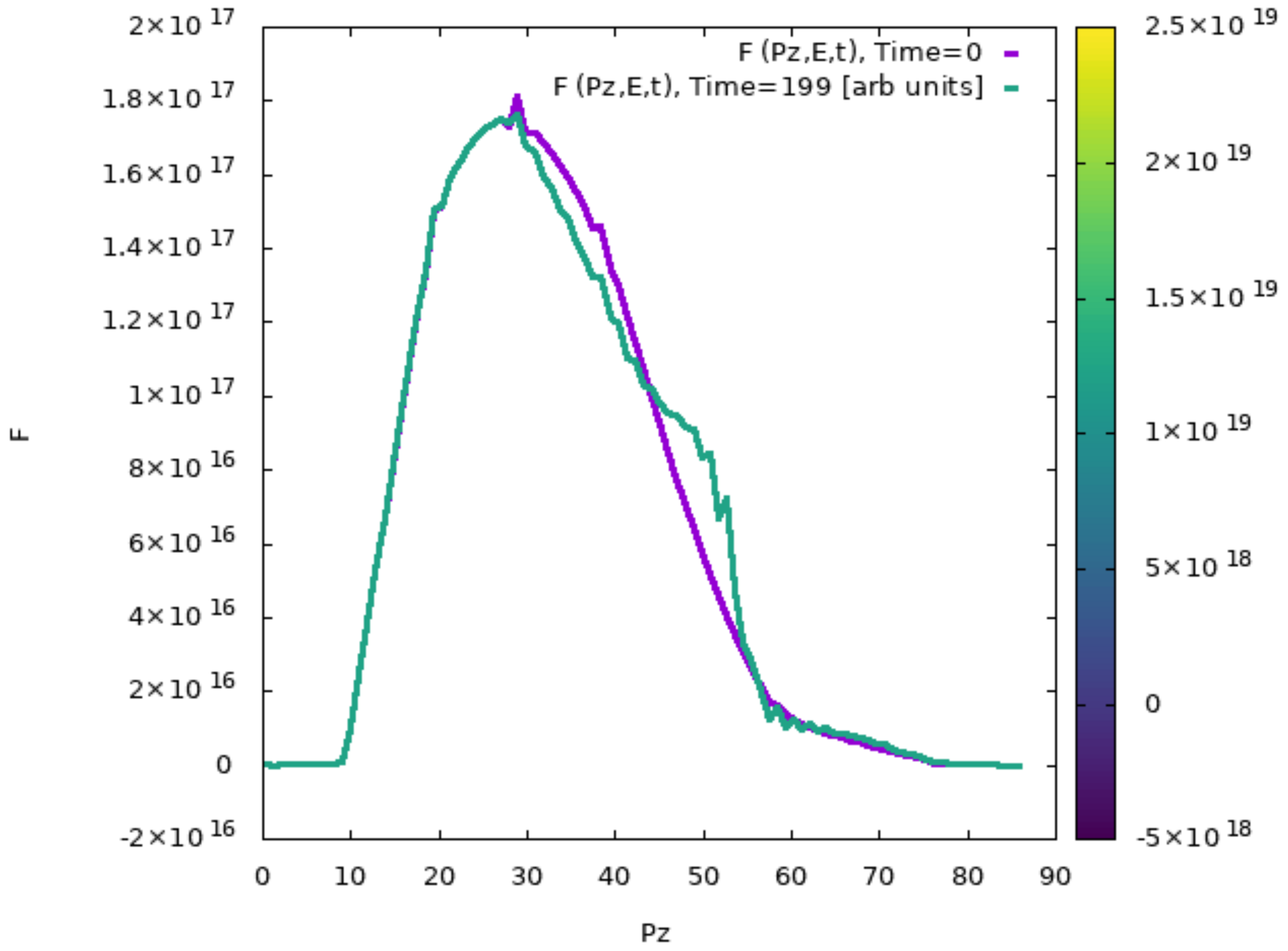


ATEP code: advance transport equation

differential dF/dt:

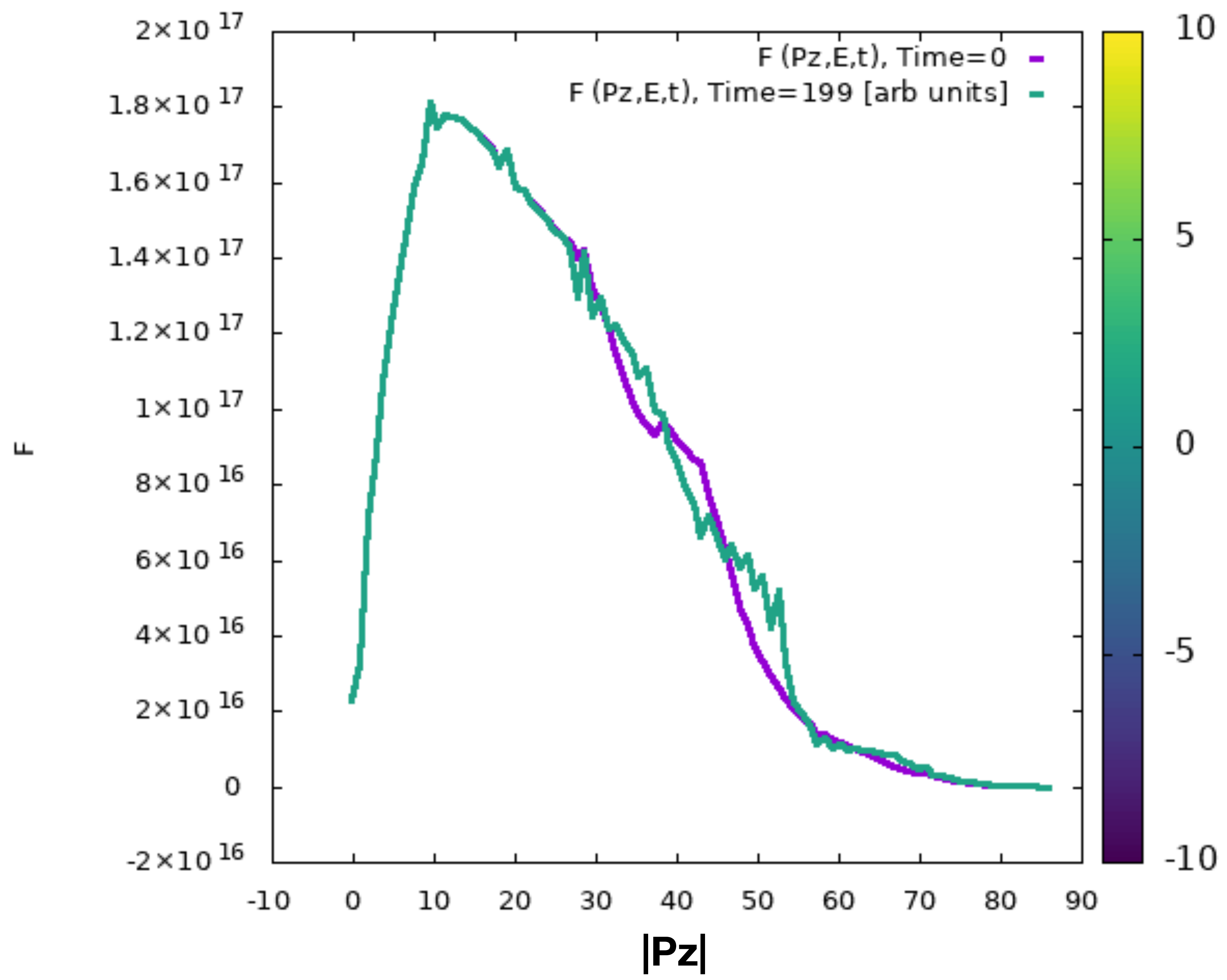


ATEP code: advance transport equation: 1d projection

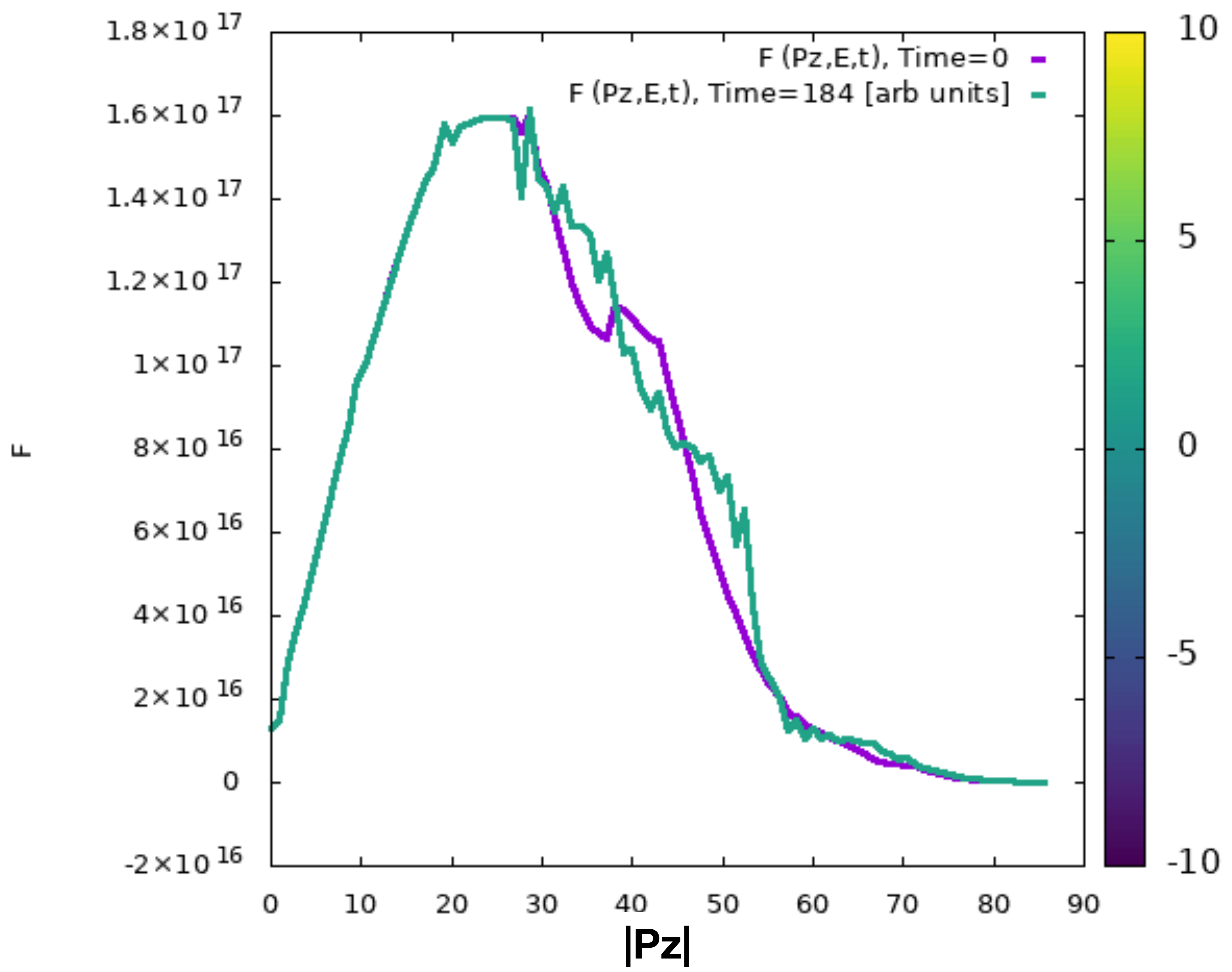


using ITER NBI off-off configuration **|Pz|**

ATEP code: advance transport equation: 1d projection



using ITER NBI on-on configuration



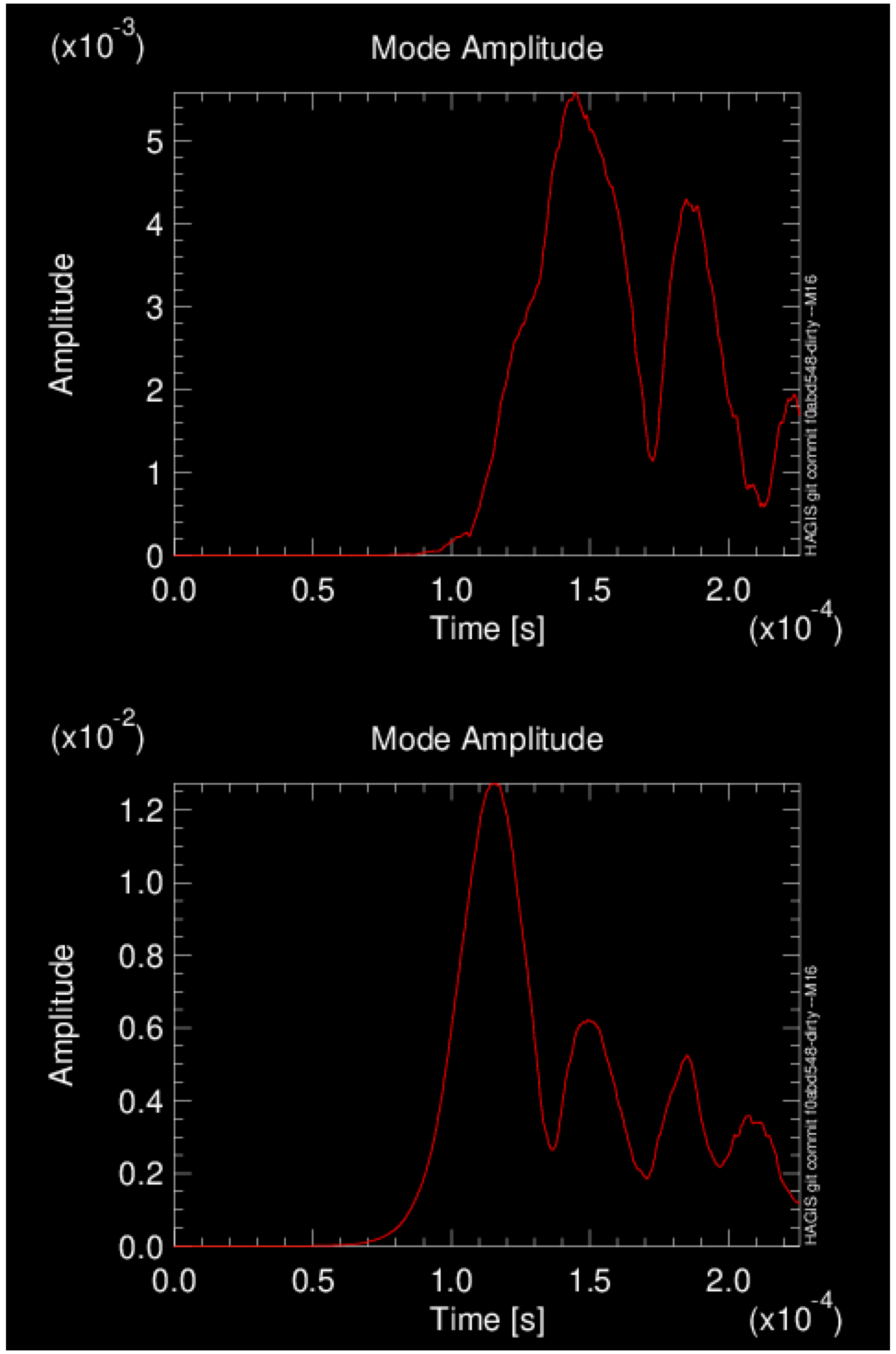
using ITER NBI on-off configuration

verification plans

- add PSZS diagnostic to post-run HAGIS output and compare F_{EP}(ATEP) and F_{EP}(HAGIS) for:

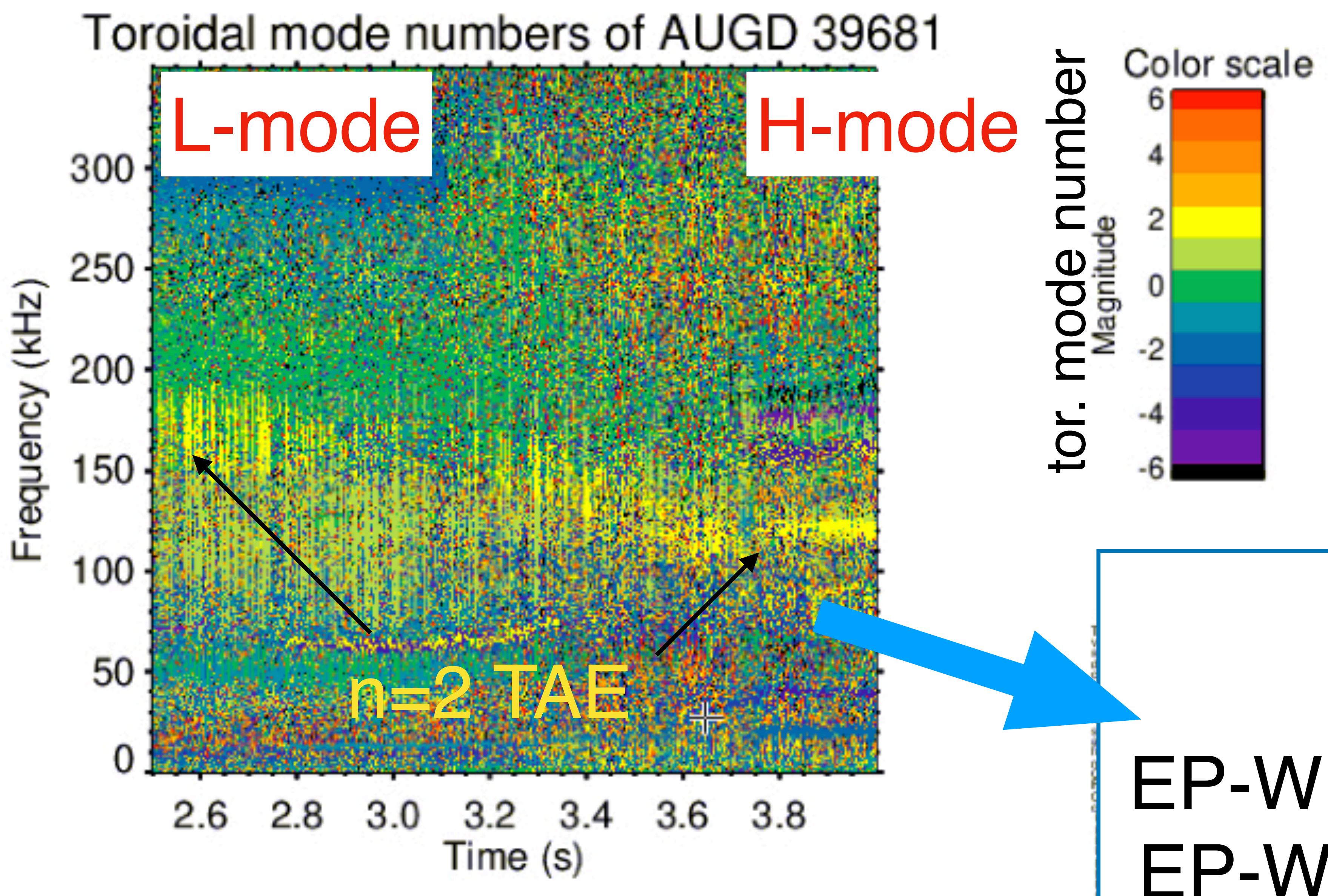
  - smoothing of F_{EP}
  - convergence of PSZS (no. orbits, resolution,etc…)
  - mode spectrum
  - Pz and E transport w/o $E_{//}$

- compare to ORB5, HMGC/HYMAGIC in various limits



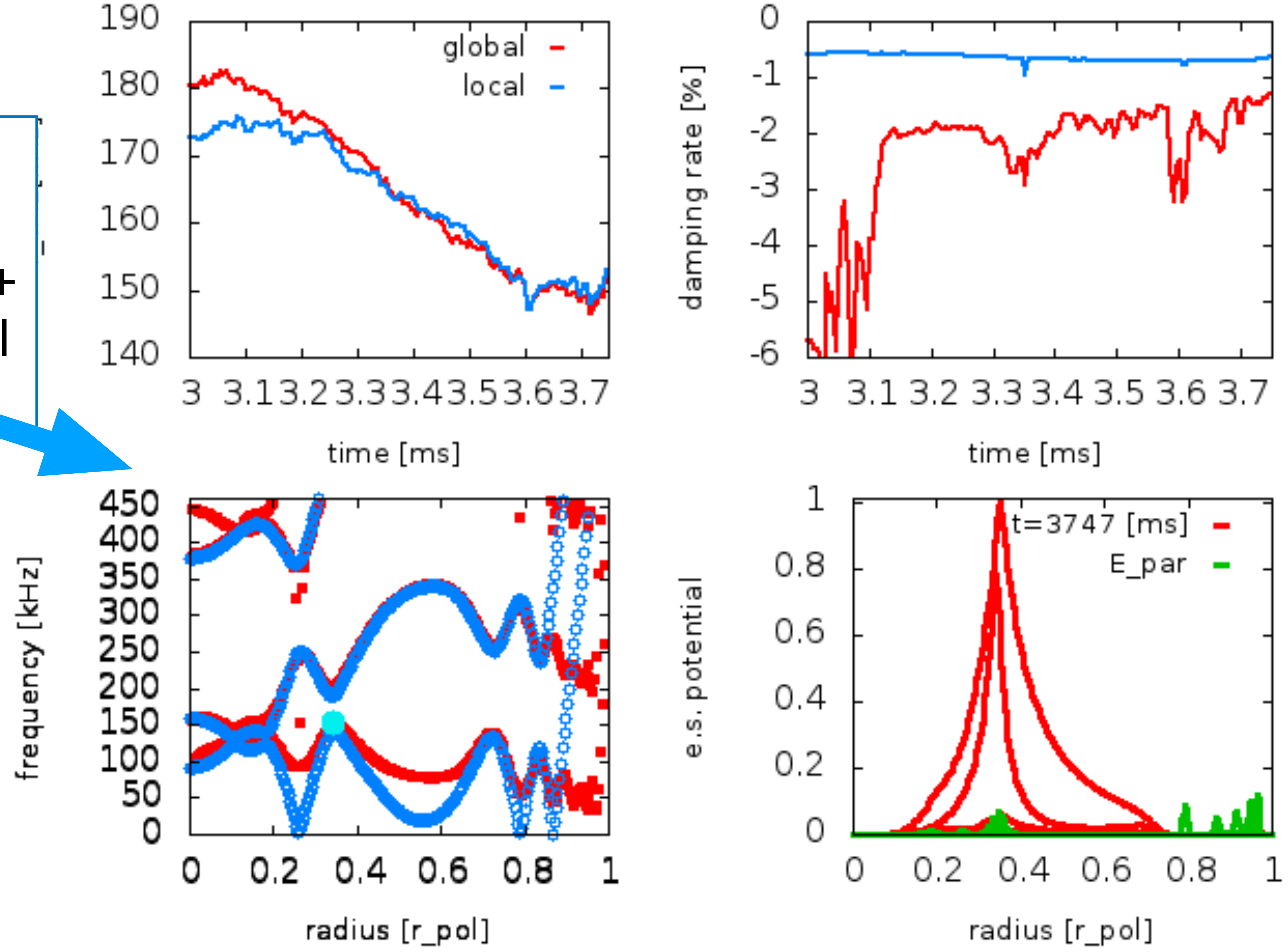
validation plans

exploit EP stability workflow: AUG data example: L-H transition in presence of TAEs



- automated processing of 160 time slices based on IDA equilibria and profiles
- fully implemented in IMAS, ensuring reproducibility

IDA +
TRVIEW +
EP-WF: LIGKA local +
EP-WF: LIGKA global

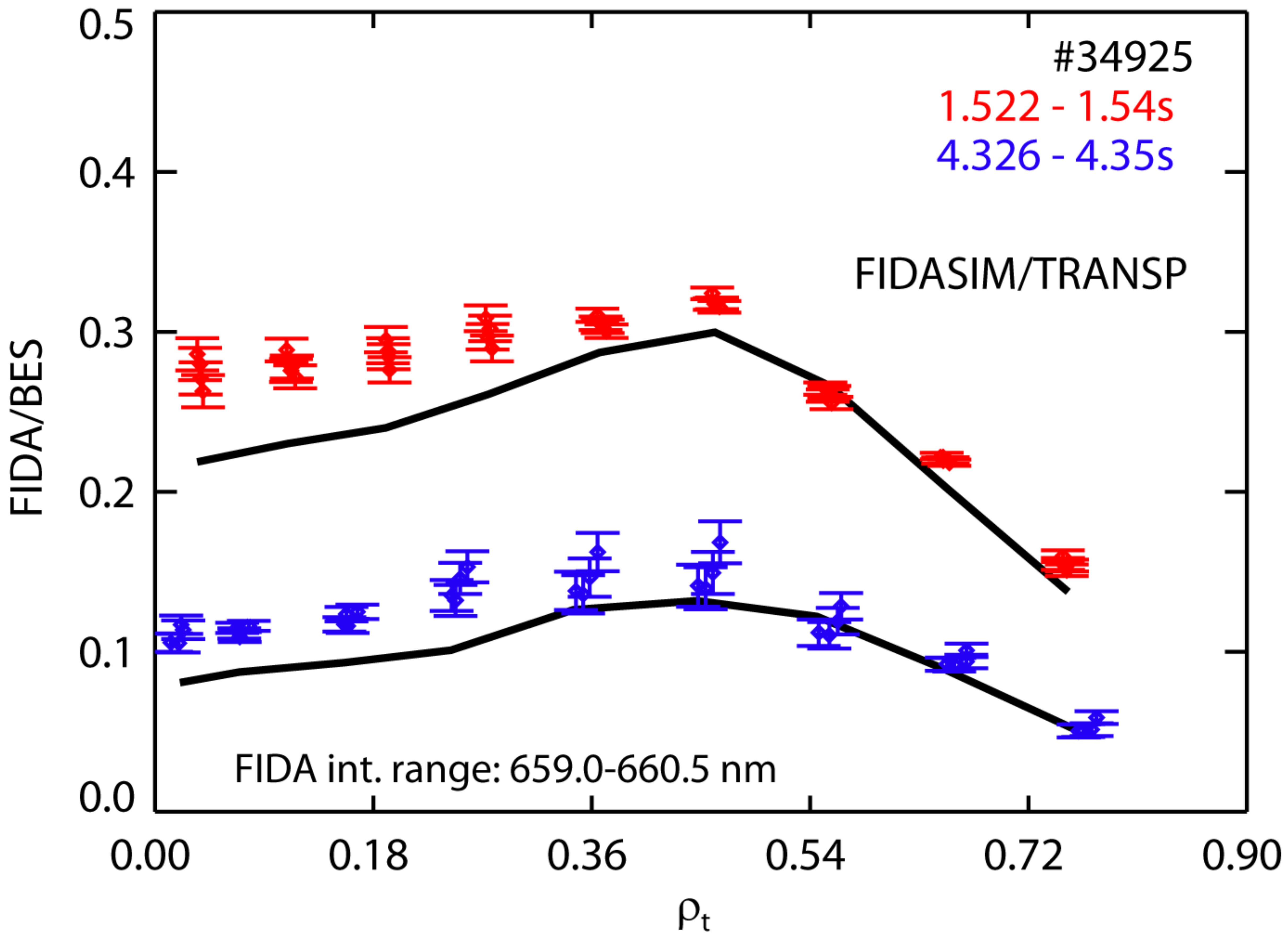


- analyse L-mode,H-mode and transition phase using
- also systematic uncertainty quantification feasible

radial flattening of EP gradient observed - inwards transport

[Lauber IAEA FEC 2018]

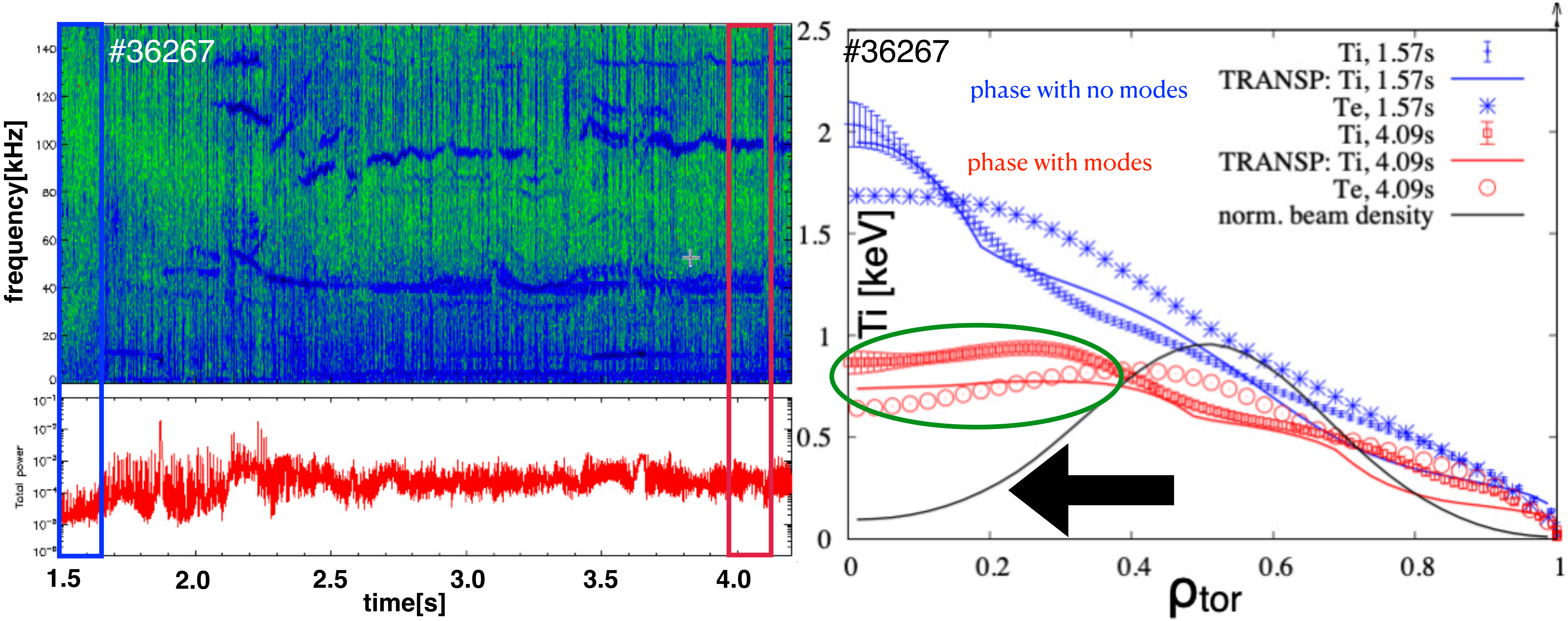
TAEs redistribute particles radially: FIDA measurements in comparison to neoclassical TRANSP/NUBEAM calculations - inwards transport due to off-axis peaked FNBI



control case available, where no strong Alfvénic mode activity is observed (#34921)

Evidence for anomalous core background ion heating due to Alfvénic modes

assess effect of EP re-distribution on Te profiles - is the transport enough to explain the Te difference?



other cases/experiments very welcome!

summary & outlook

- IMAS-based orbits data-base and QL orbit averaged particle response implemented - PSZS structures stored as IDS distribution objects

- general F_{EP} generated from marker data

- evolved PSZS transport equation in kick-model limit

next steps:

- fill transport IDS with D(s,E) - couple to RABBIT/ETS
- add amplitude dependence of PSZS i.e. d (dP/dt)dPz * F_{EP} term -> similar to RBQ model
- add various intensity closure models
- add collisions and sources - starting with Langevin limit for decorrelation processes, add bounce averaged collision operators - compare with CKA-EUTERPE [Brizard, Slaby/Kleiber, Hoppe,…]
- can be used to check diffusive vs convective model, different mode spectra, overlap criteria
- separate scales according to PSZS theory -> use to evolve to non-linear equilibria

- speed up, hopefully ACH support next year, integrate in WF framework