



On the development of advanced energetic particle transport models

3rd Trilateral International Workshop on EP physics, 10.11.2022

Ph. Lauber, V.-A. Popa, T. Hayward-Schneider, G. Meng, 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/>



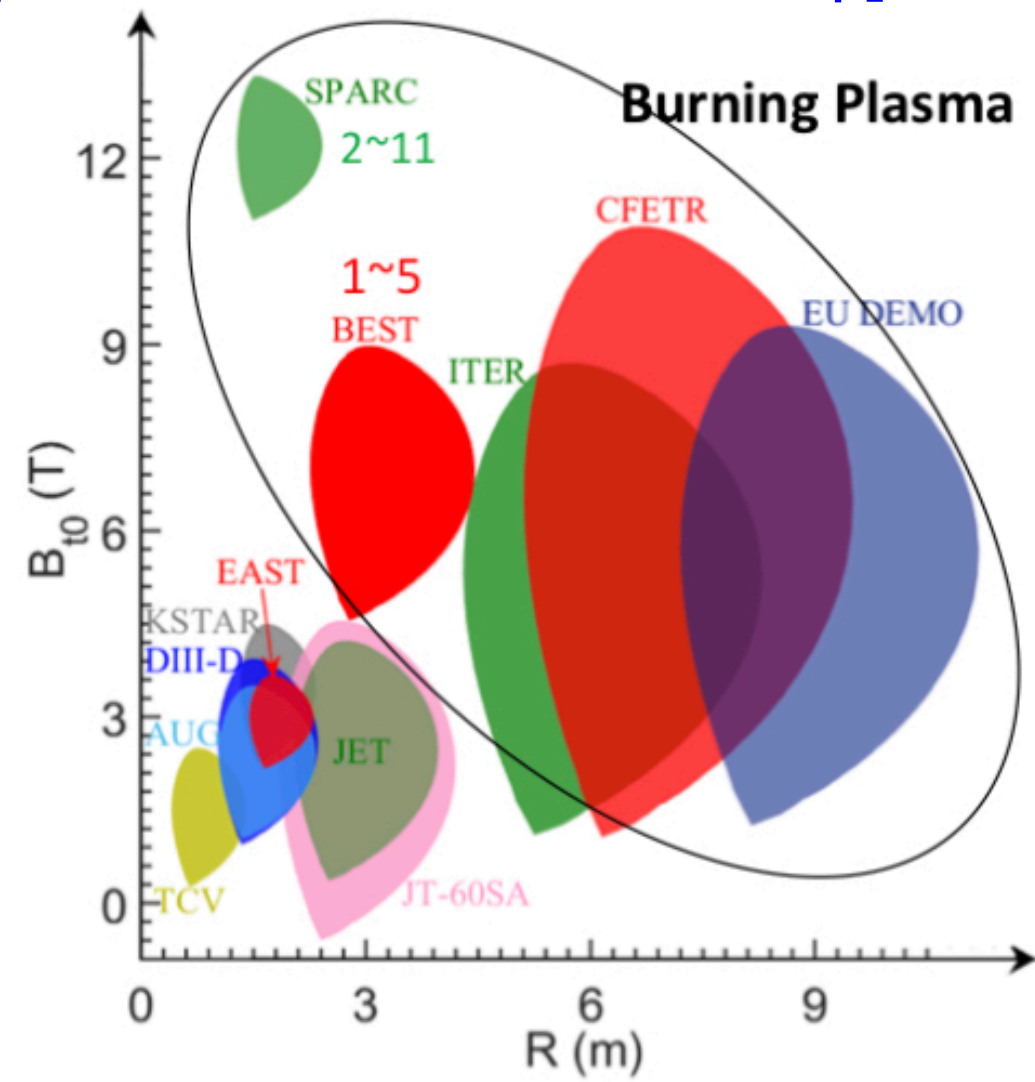
MAX-PLANCK-INSTITUT
FÜR PLASMAPHYSIK



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[Baonian Wan, at this workshop]

for scaling from TCV-AUG-JET,... to JT-60SA-DTT-ITER-DEMO-any other other device, we need:



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 e.m.

linear global kinetic e.m.

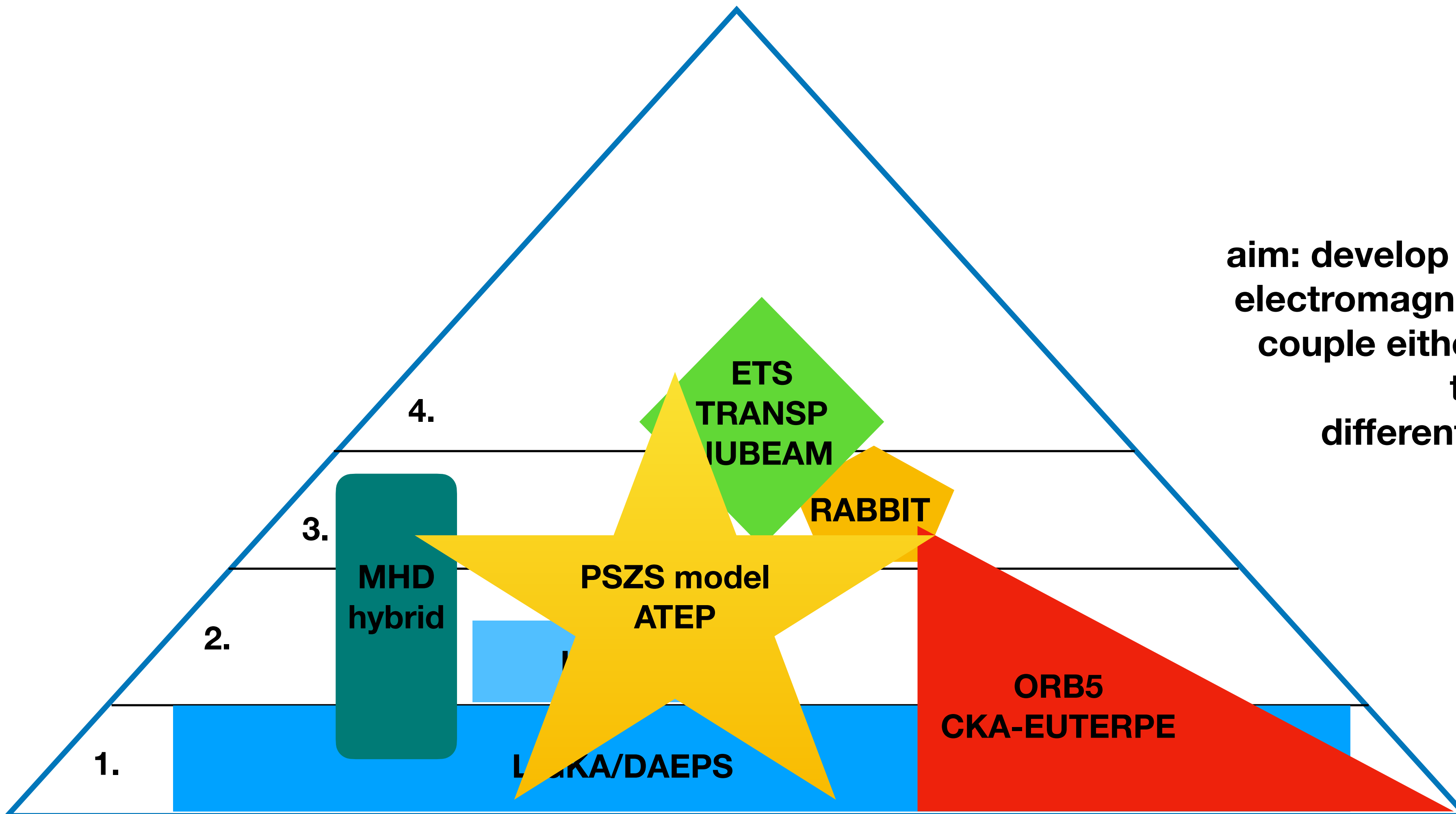
4. self-organisation - back reaction of EP transport on profiles and background transport

3. EP transport and losses

2. non-linear mode evolution, saturation mechanisms

1. mode stability

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

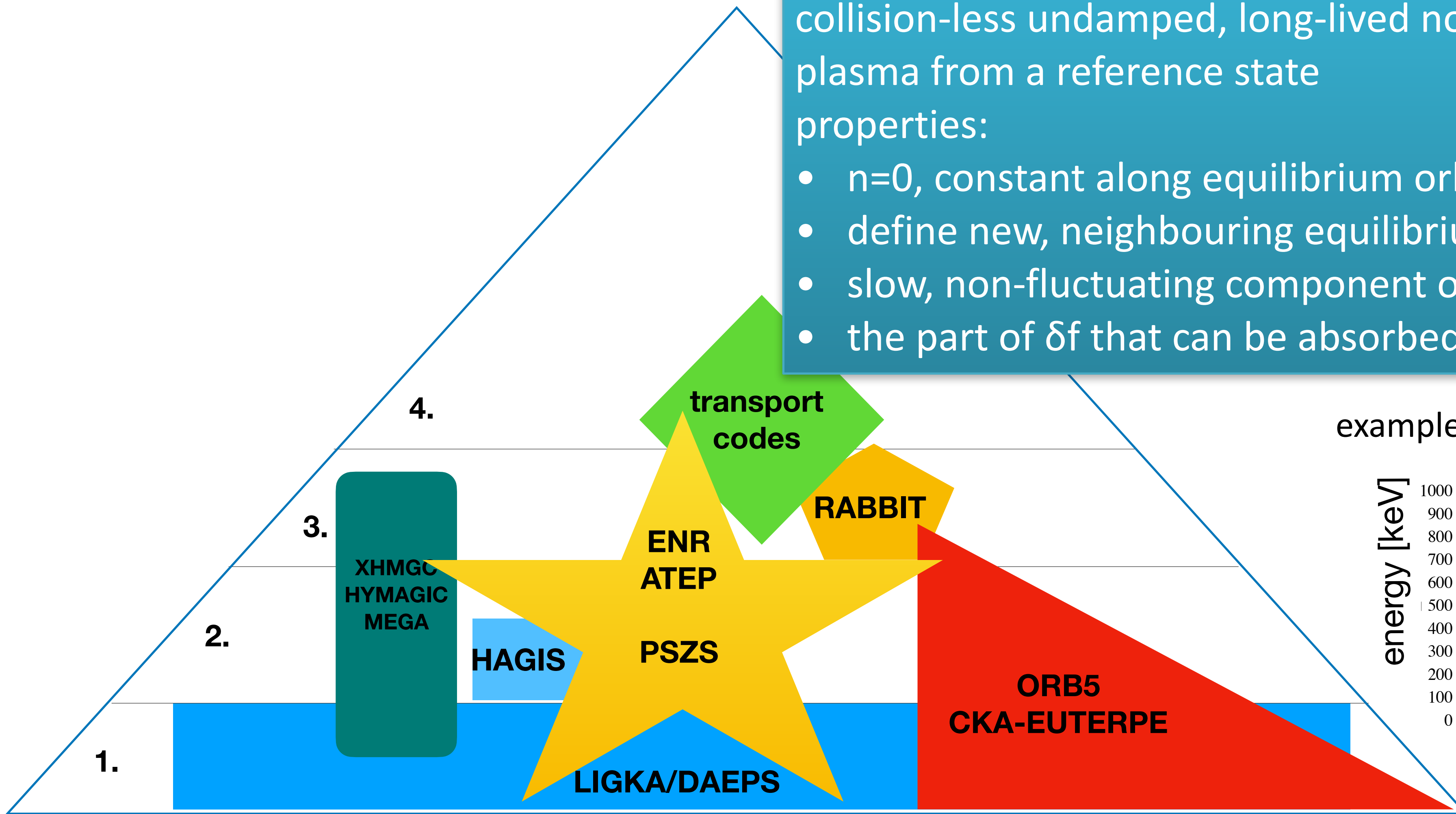


aim: develop IMAS based tool to calculate electromagnetic, global EP transport and couple either via F_{EP} or its moments to transport codes; different models of fidelity/cost

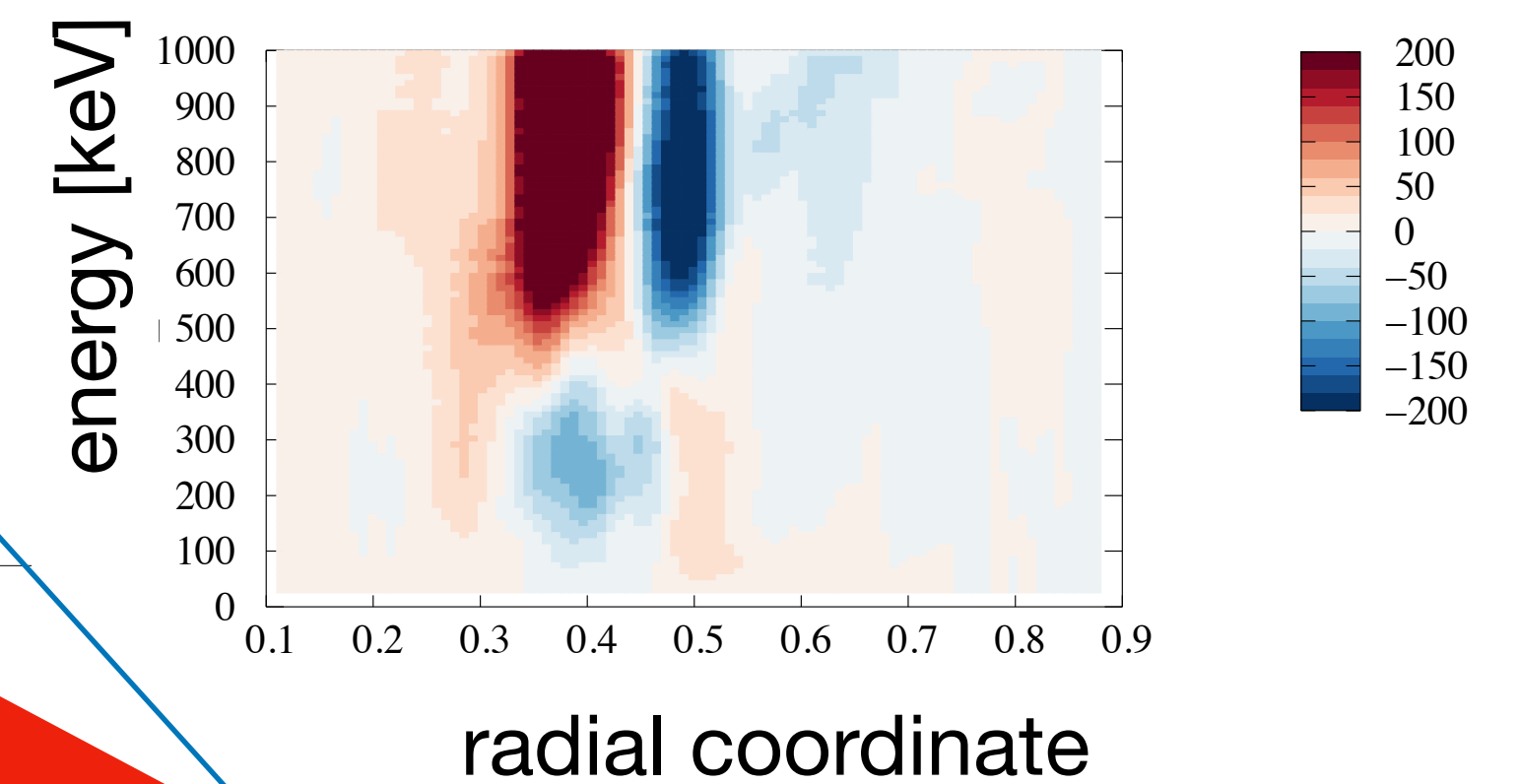


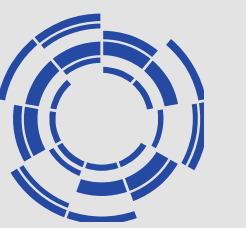
phase space zonal structures (PSZS) are : [see M. Falessi's talk at this workshop]
 collision-less undamped, long-lived nonlinear deviations of the plasma from a reference state
 properties:

- $n=0$, constant along equilibrium orbits
- define new, neighbouring equilibrium reference state
- slow, non-fluctuating component of F_{EP} evolution
- the part of δf that can be absorbed in new F_0



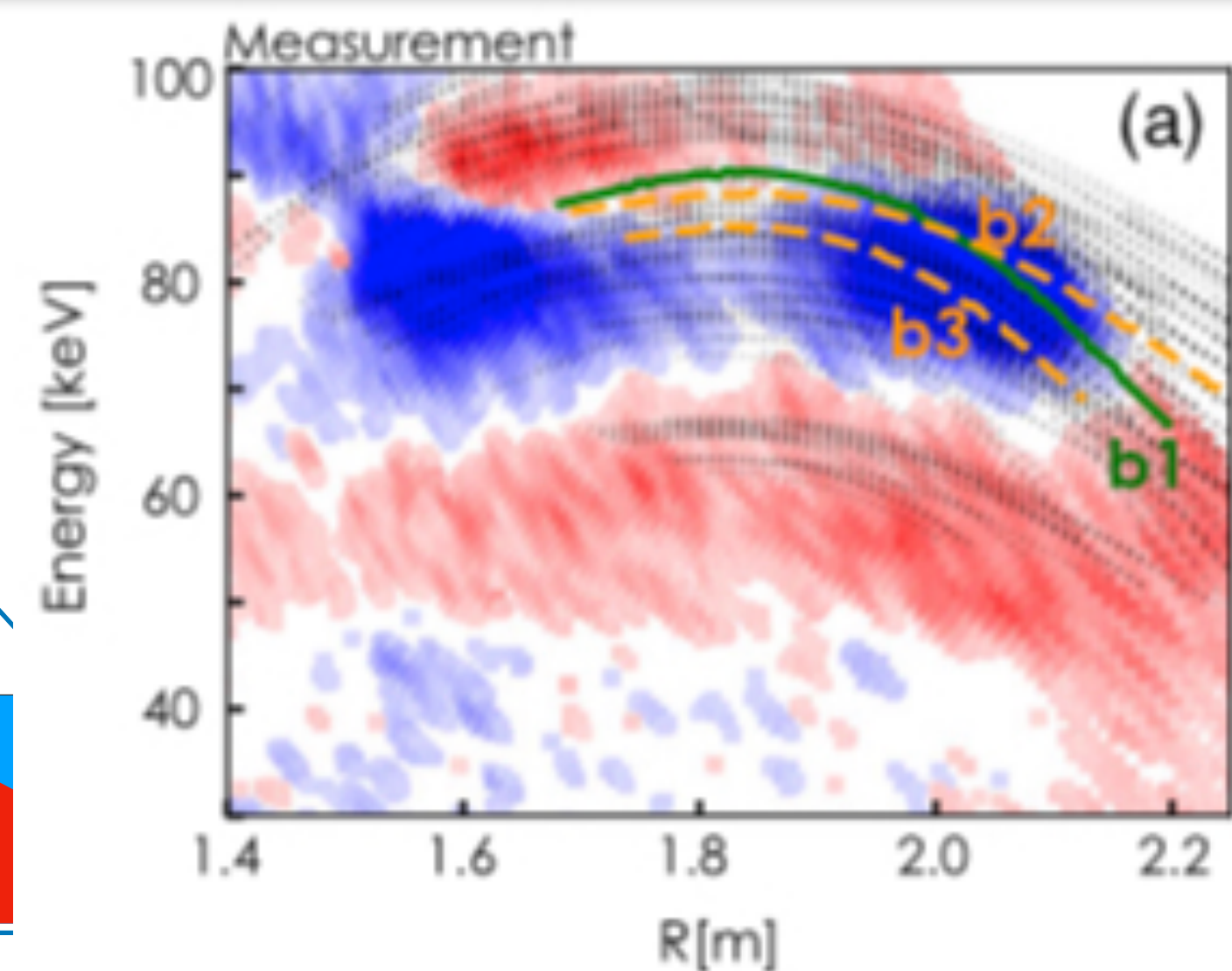
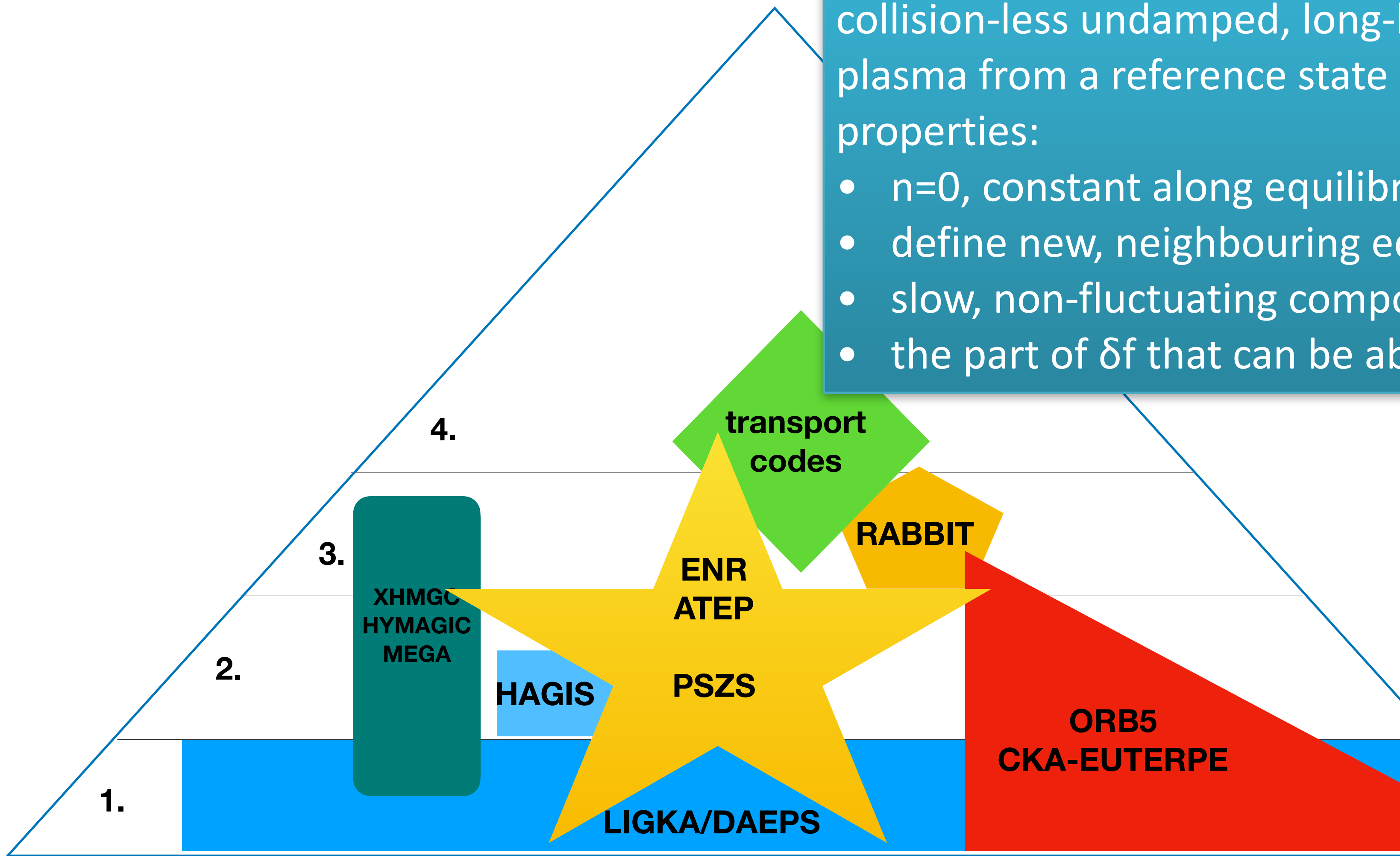
example in COM space representation:





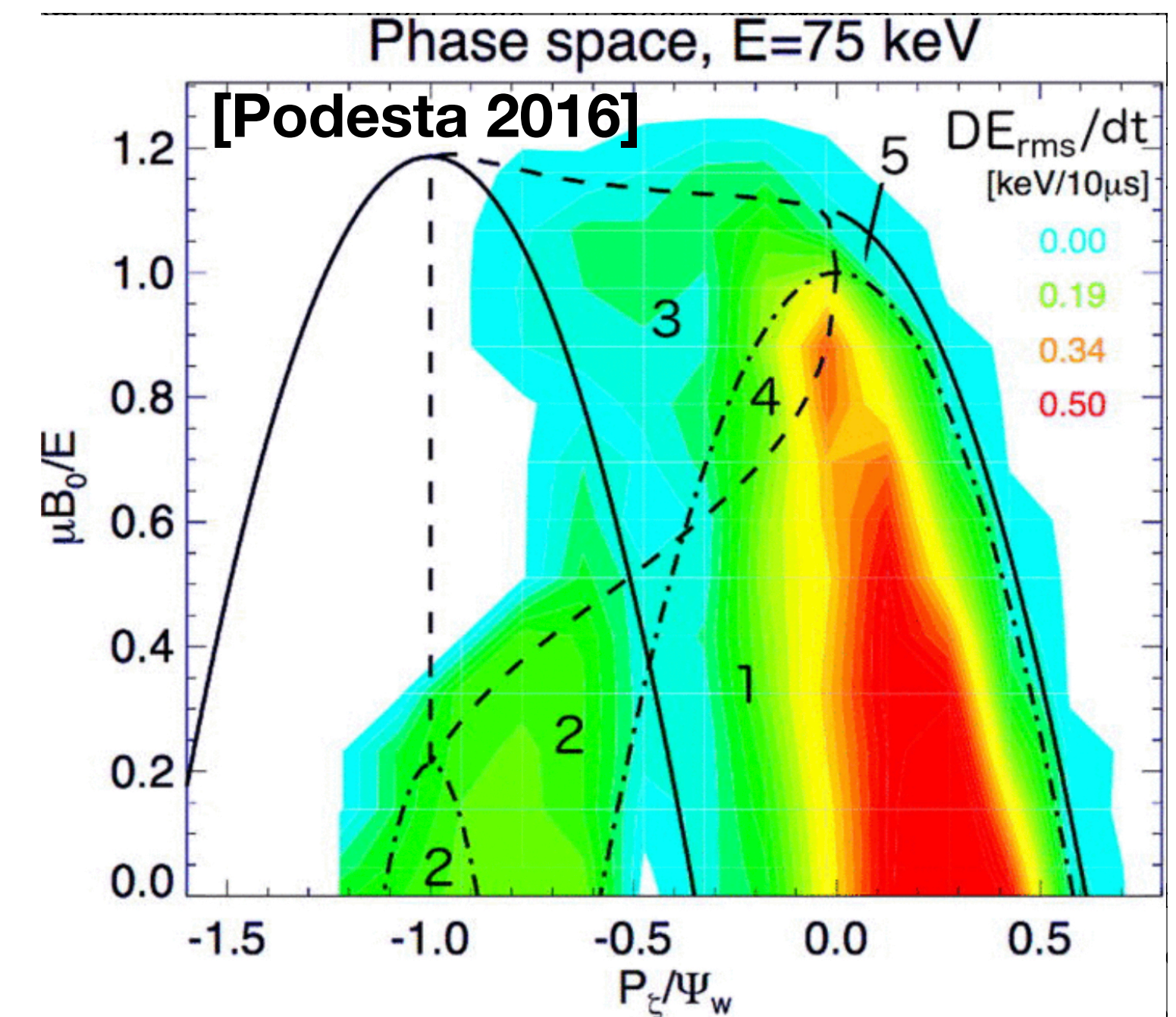
phase space zonal structures (PSZS) are : [see M. Falessi's talk at this workshop]
 collision-less undamped, long-lived nonlinear deviations of the plasma from a reference state
 properties:

- $n=0$, constant along equilibrium orbits
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DIII-D, INPA [Du et al PRL 2021]

- diffusion coefficients for impurity transport by background turbulence, no e.m. EP-driven modes [Angioni, Püsichel, etc]
- critical gradient model [R. Waltz, E. Bass]: use local AE stability threshold, add upshift of transport threshold using $(ExB)_{\text{turb}}$ shearing rate; above threshold set DEP to ad hoc values [e.g. $10\text{m}^2/\text{s}$] to clamp EP's radial gradient to critical value
- kick model [M. Podesta, 2014-2022]: calculate probability density function of kick in P_z 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, 2017-2022] - 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



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

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

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]

$$\begin{aligned} \frac{\partial}{\partial t} (B_{\parallel}^* F_o) + \bar{\nabla} \cdot (B_{\parallel}^* \dot{X}_o F_o) + \frac{\partial}{\partial \mathcal{W}} (B_{\parallel}^* \mathcal{W}_o F_o) + \bar{\nabla} \cdot (B_{\parallel}^* \delta \dot{X} \delta G_{res}) \\ + \frac{\partial}{\partial \mathcal{W}} (B_{\parallel}^* \delta \dot{\mathcal{W}} \delta G_{res}) = 0 \end{aligned} \quad (12)$$

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

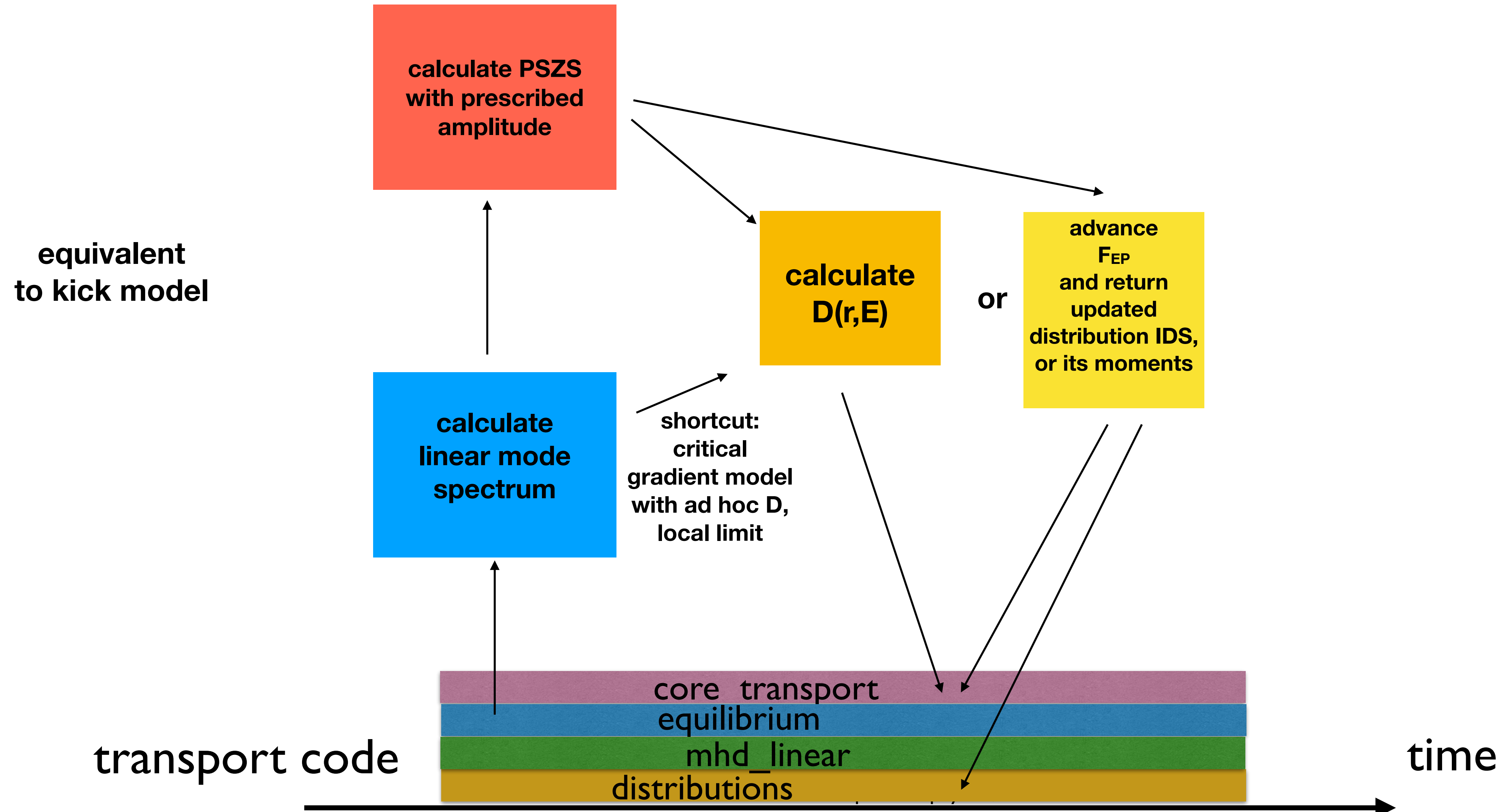
$$D_{\psi\psi} = \overline{\delta\psi\delta\psi} \tau_{ac} = \frac{1}{2} \sum_{\omega, \mathbf{k}_\perp} c^2 m_\beta^2 |\delta\hat{\Phi}|^2 \tau_{ac} \quad (45)$$

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

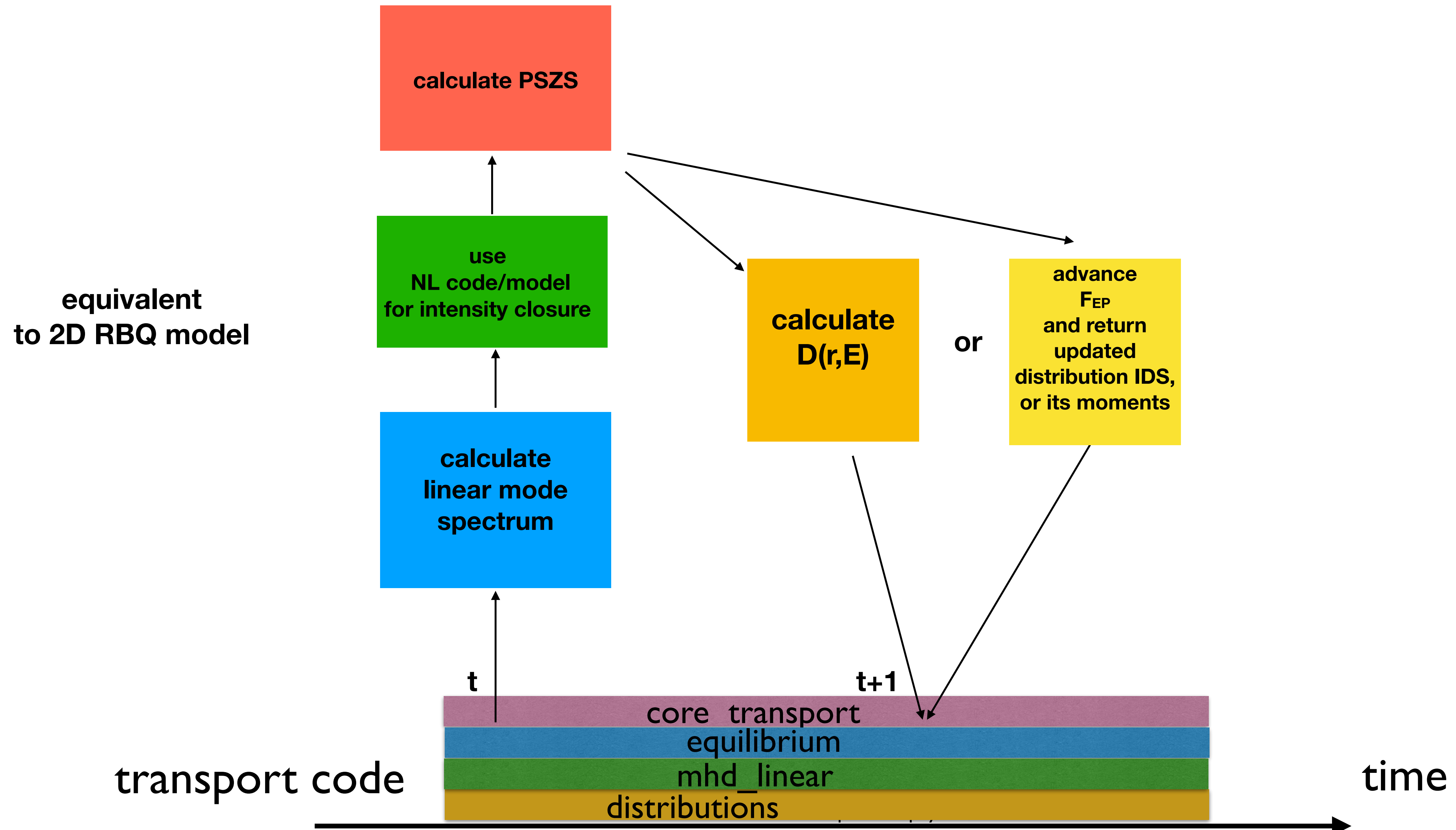
$$D_{\epsilon\epsilon} = \overline{\delta\dot{\epsilon}\delta\dot{\epsilon}} \tau_{ac} = \frac{1}{2} \sum_{\omega, \mathbf{k}_\perp} \left(\frac{\omega e}{m} \right)^2 |\delta\hat{\Phi}|^2 \tau_{ac} \quad (47)$$



outline: ATEP framework EP transport workflow schematics

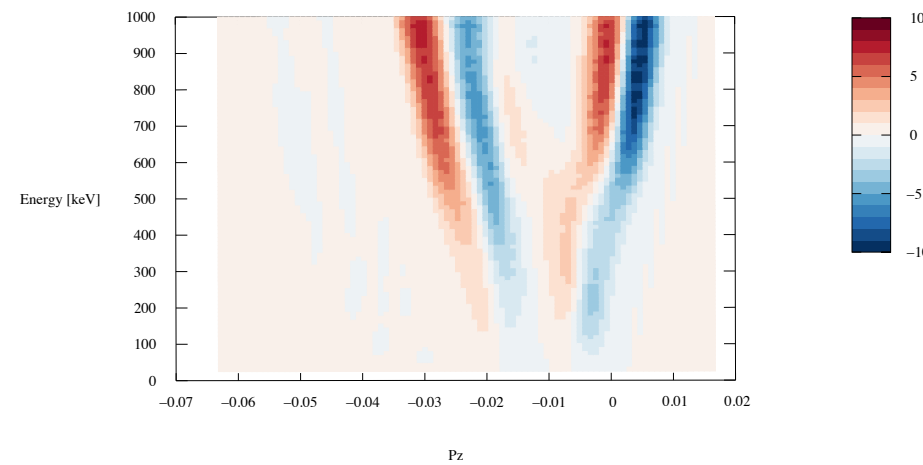


EP transport workflow schematics



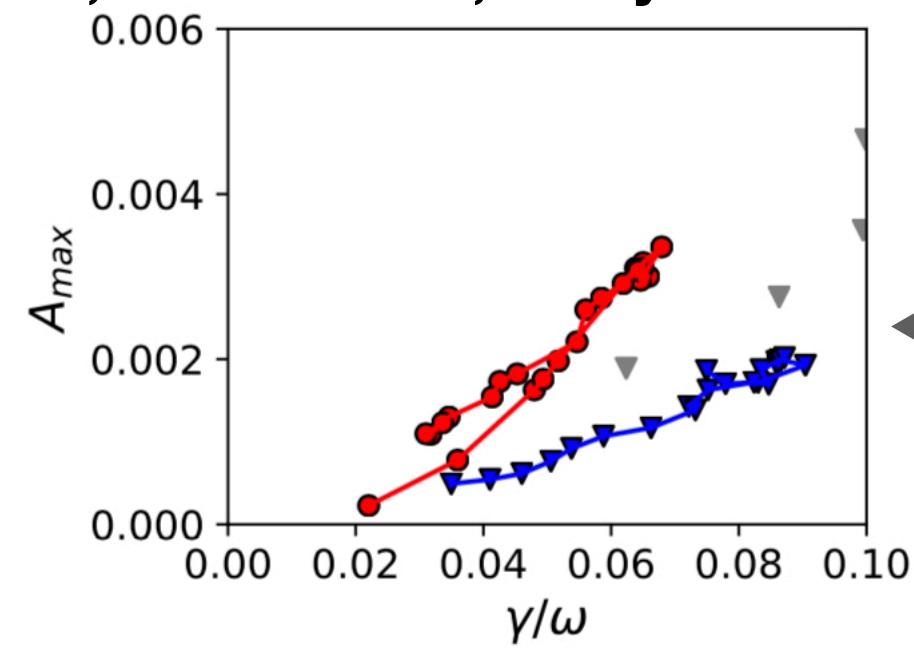
EP transport workflow schematics

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



calculate PSZS

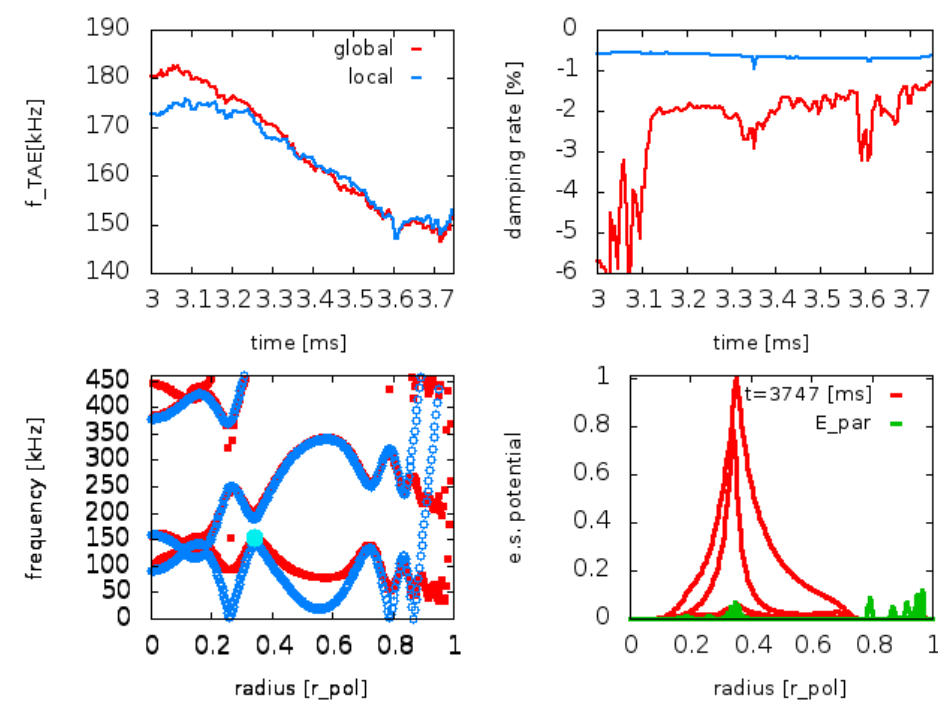
[HAGIS, S.D. Pinches, T Hayward-Schneider]



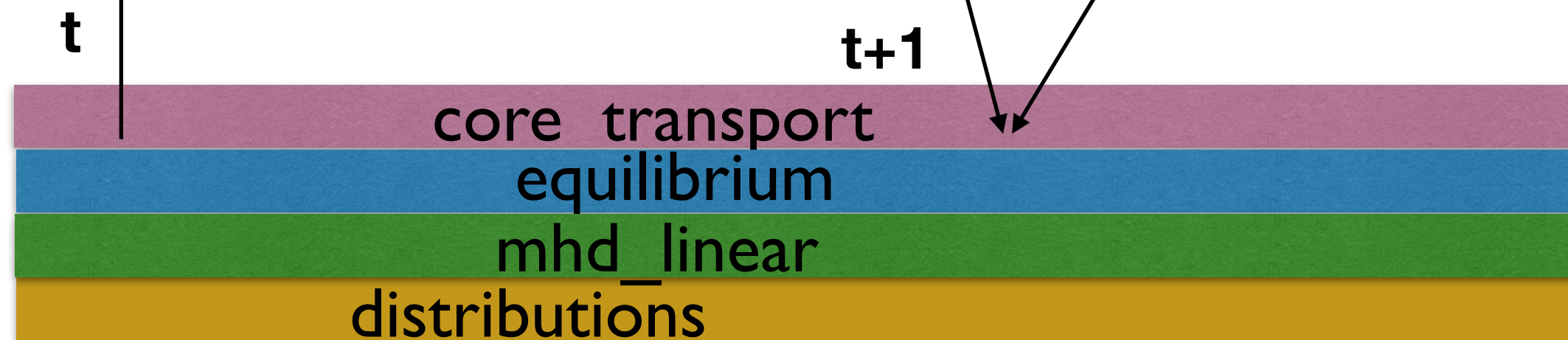
use
NL code/model
for intensity closure

calculate
linear mode
spectrum

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



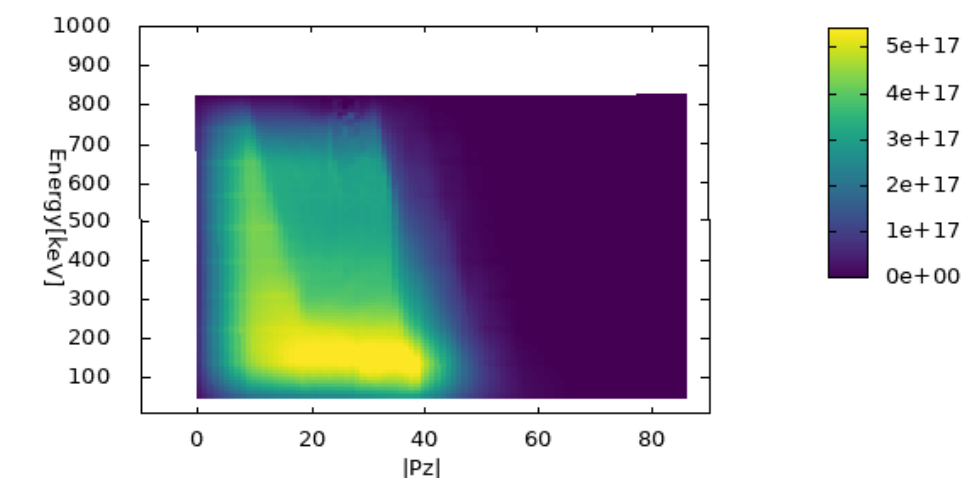
transport code



time

ATEP code [Ph. Lauber, 2022]

F(Pz,E,t), Time=199 [arb units]



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



- **Linear stability: EP stability**
- **calculating PSZSs**
- **progress on implementation of transport model: ATEP code**
- **verification & validation**

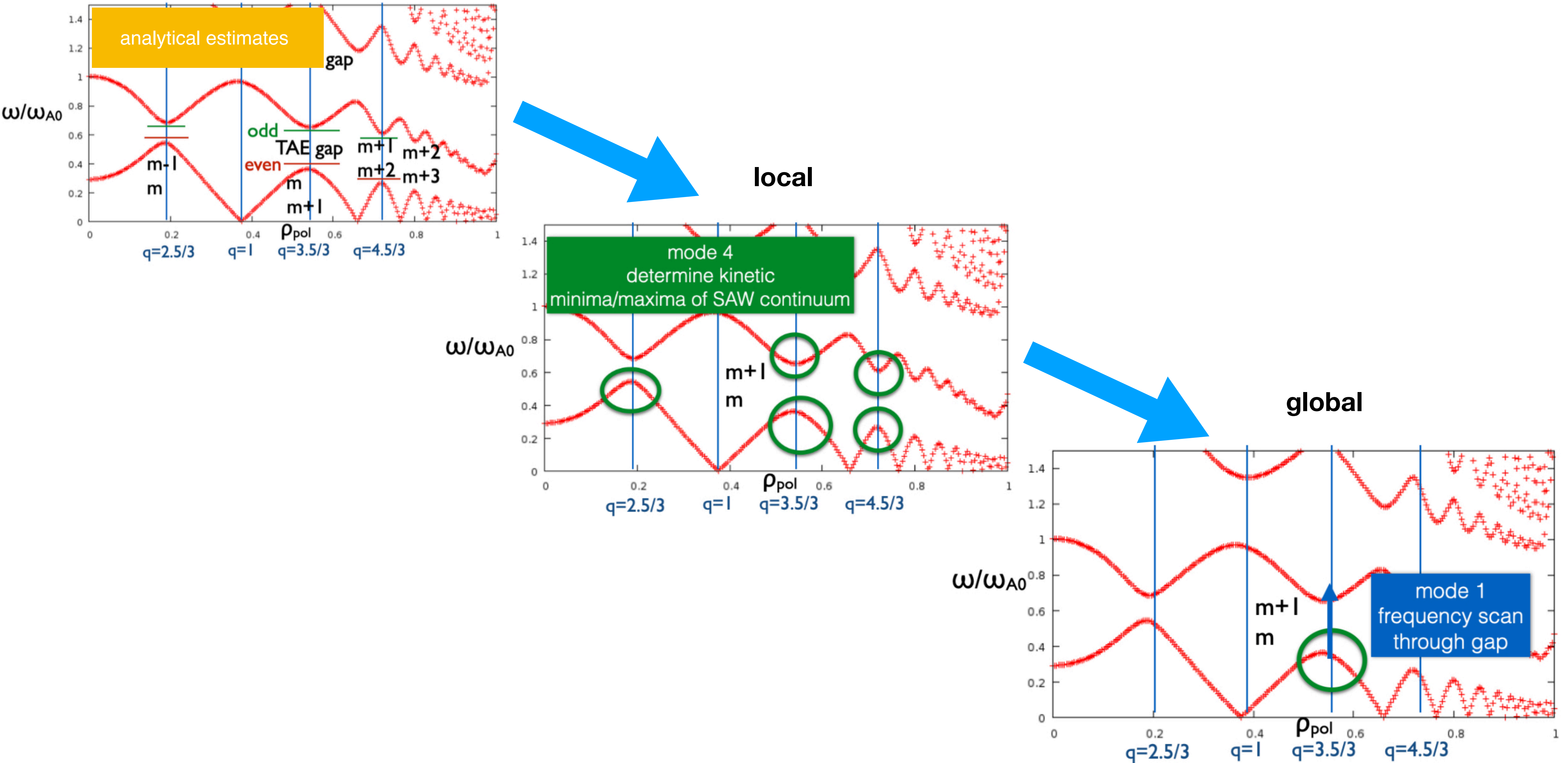
- local, analytical estimates [mode 5]
- local reduced MHD - spectra [mode 6]
- global reduced MHD - MHD eigenfunction [mode 6]
- local kinetic (w/o numerical coefficients) [mode 3/4]
- local kinetic with FLR/FOW (w/o numerical coefficients) [mode 3/4]
- global kinetic (w/o numerical coefficients): two different solvers [mode 1]
- global kinetic track mode (w/o numerical coefficients) [mode 2]

typically modes are called in sequence;

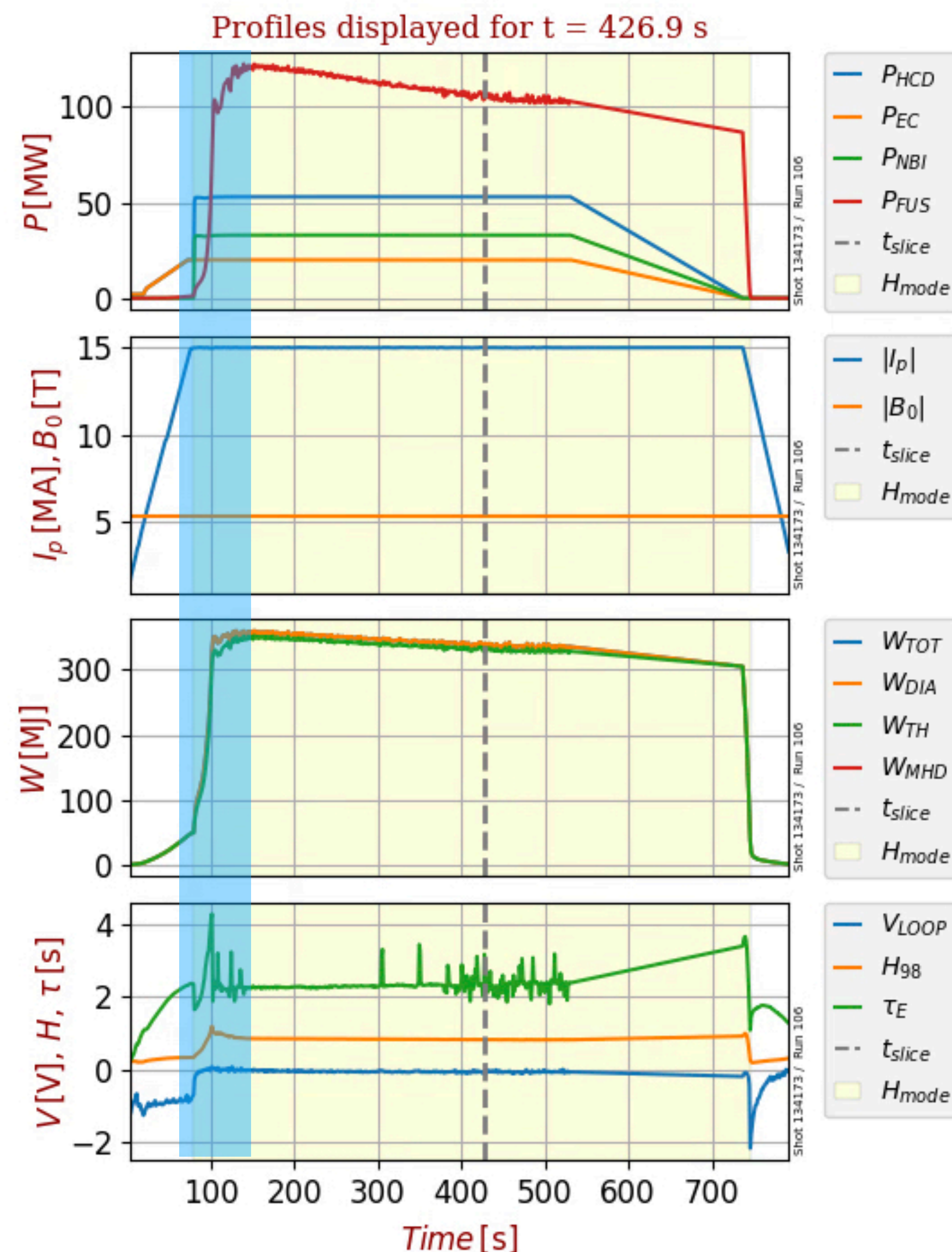
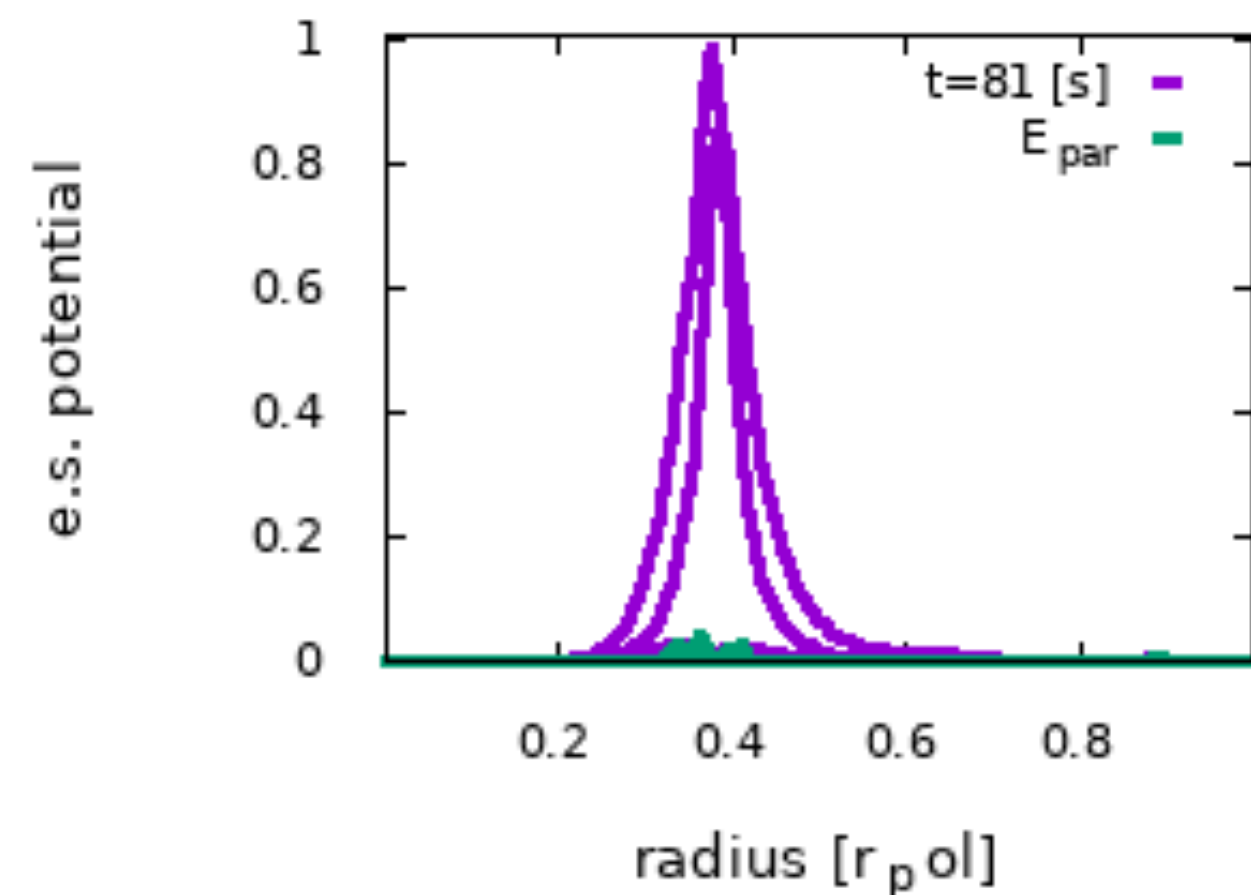
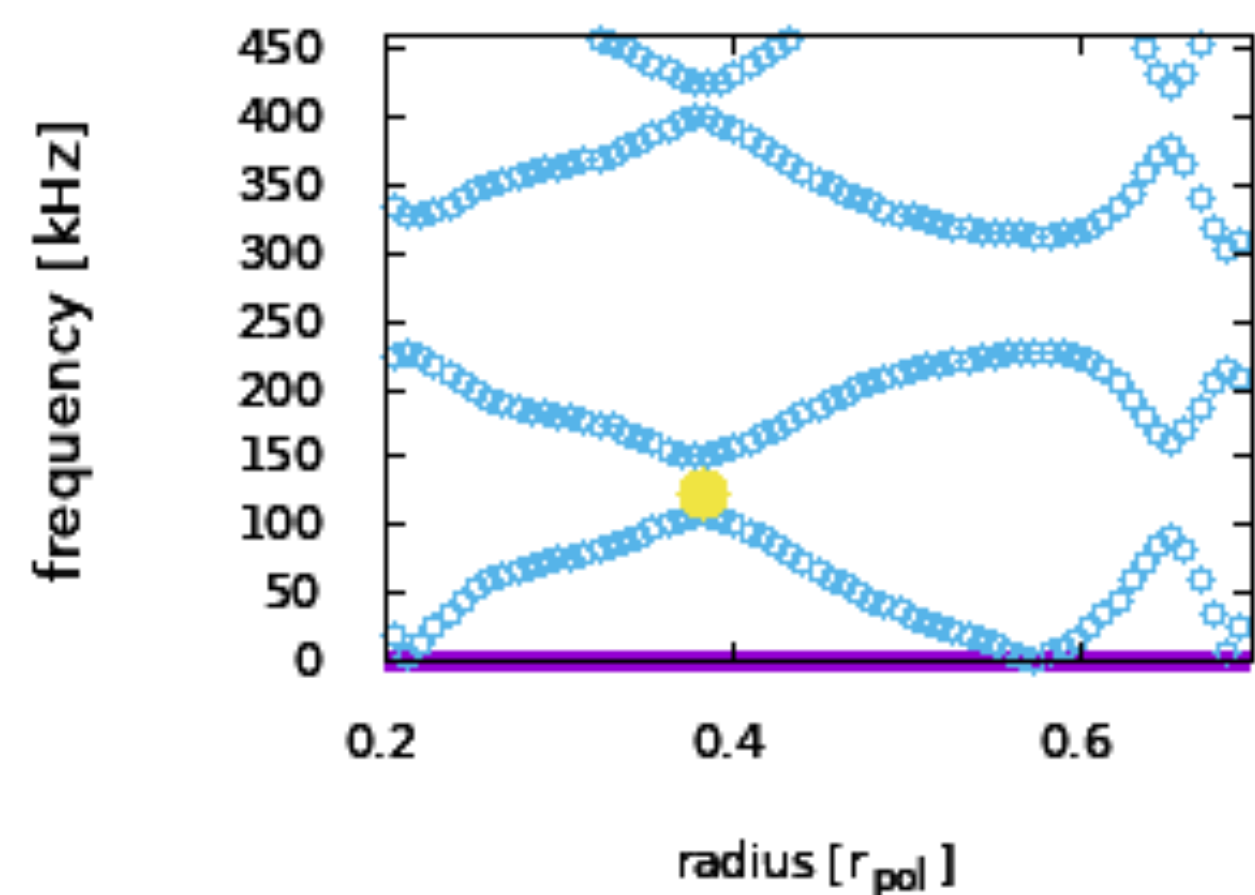
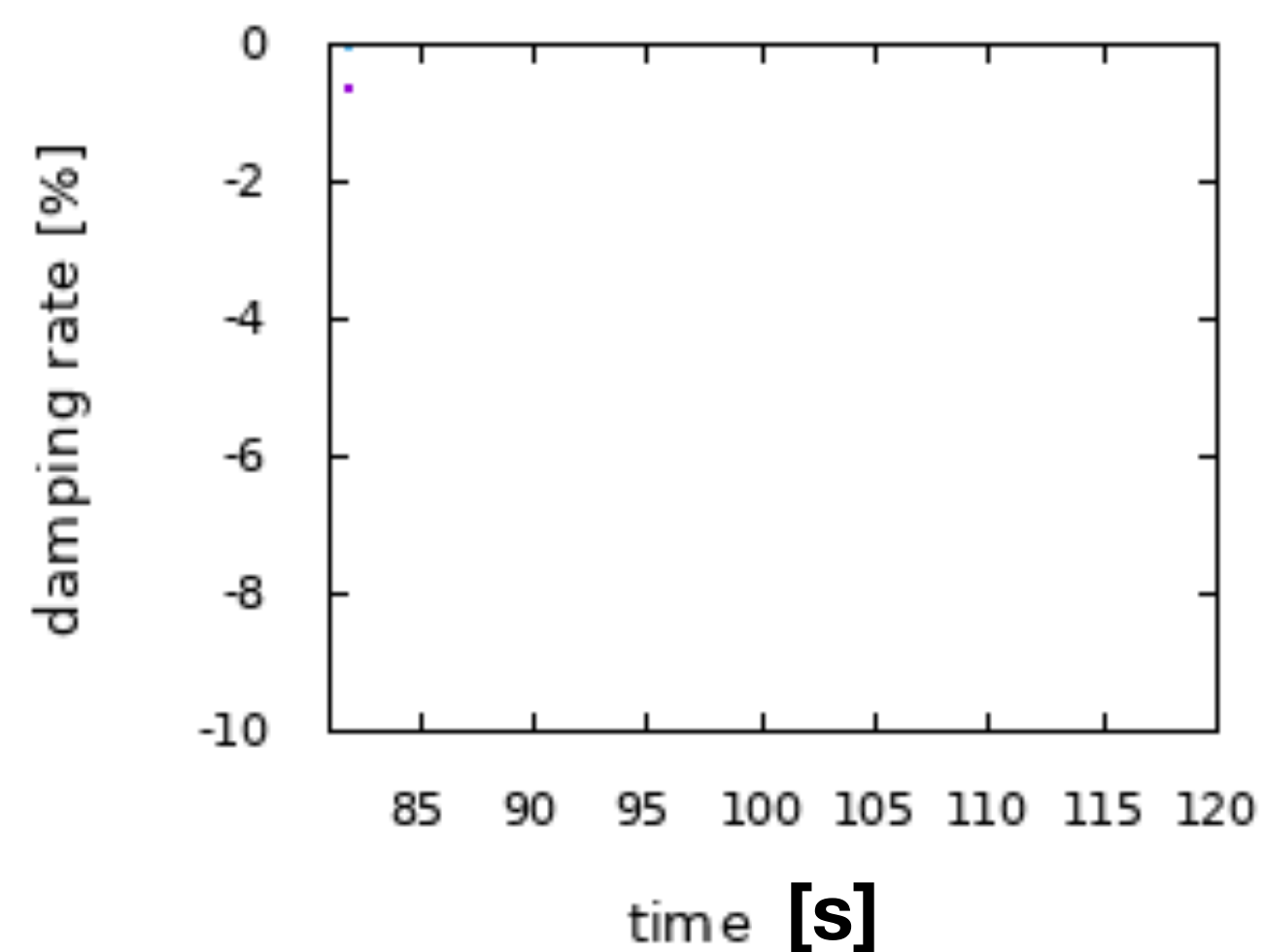
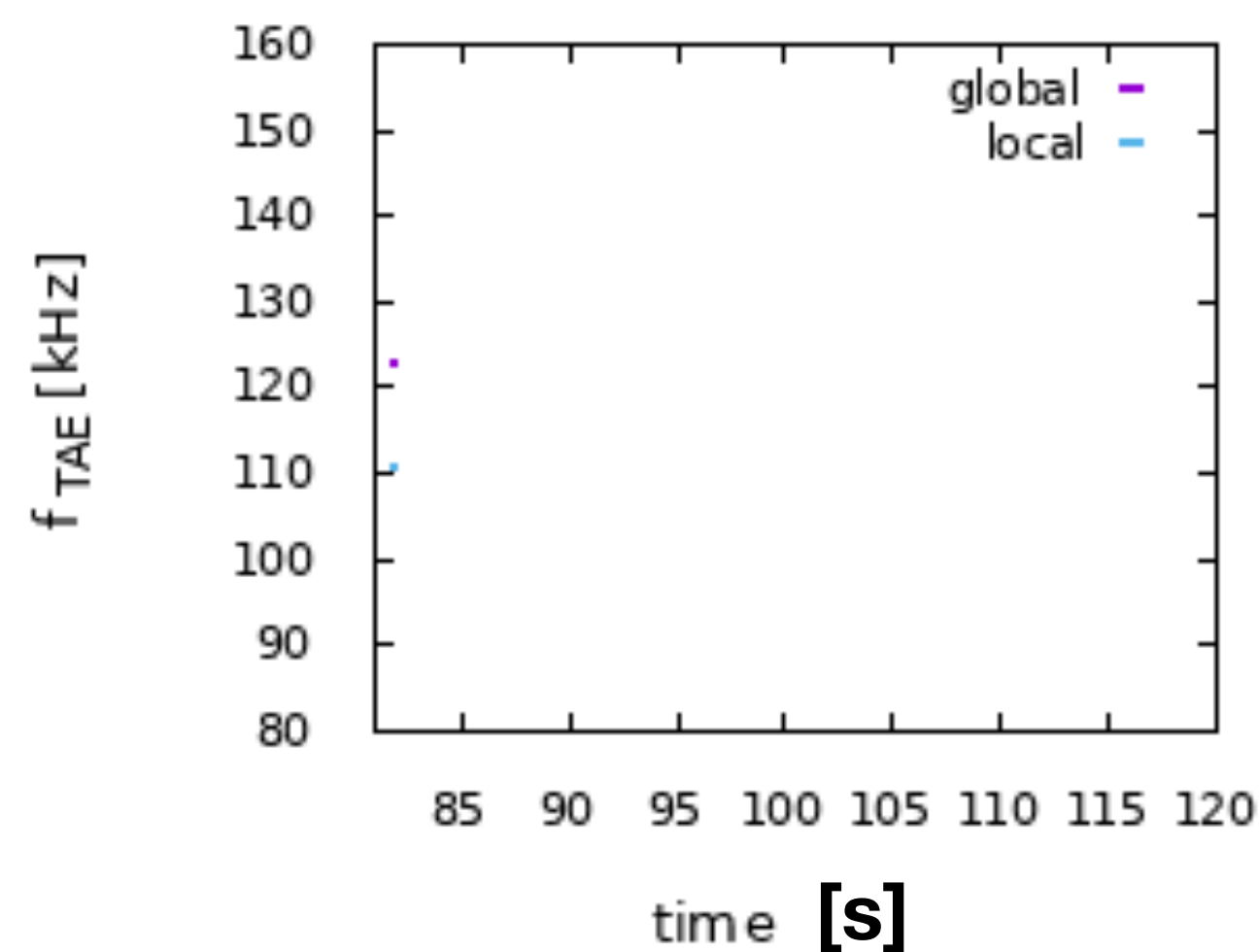
results are stored in unique structure keeping results from various calls in the same format -
adoption to IMAS finished, documentation on <https://confluence.iter.org/pages/viewpage.action?pageId=289069024>

- Lauber PhD Thesis 2003: <http://nbn-resolving.de/urn/resolver.pl?urn:nbn:de:bvb:91-diss2003111814131>
 - Lauber JCP 2007: [10.1016/j.jcp.2007.04.019](https://doi.org/10.1016/j.jcp.2007.04.019)
 - Lauber PPCF 2009: <http://stacks.iop.org/0741-3335/51/i=12/a=124009>
 - Lauber PREP 2013: <https://doi.org/10.1016/j.physrep.2013.07.001>
 - Bierwage NF 2017: <https://doi.org/10.1088/1741-4326/aa80fe>
 - Lauber JPC 2018 <https://doi.org/10.1088/1742-6596/1125/1/012015>
 - ITPA EP: <https://sharepoint.iter.org/departments/POP/ITPA/EP/Pages/default.aspx>
 - more information: <http://www2.ipp.mpg.de/~pwl/>
- and git ITER repository: `git clone ssh://git@git.iter.org/stab/ligka.git` ; git checkout develop

use local information for setting up global simulation

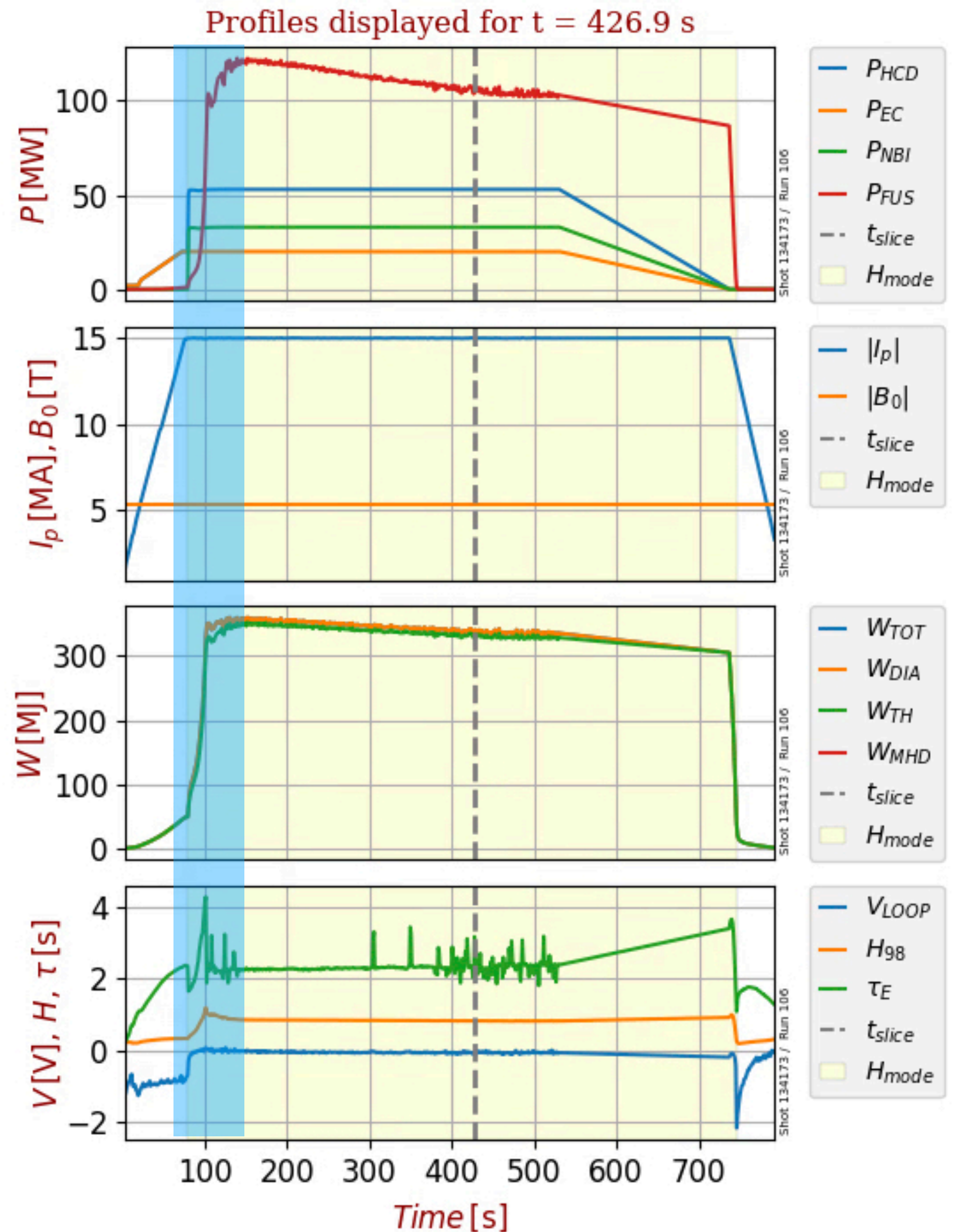
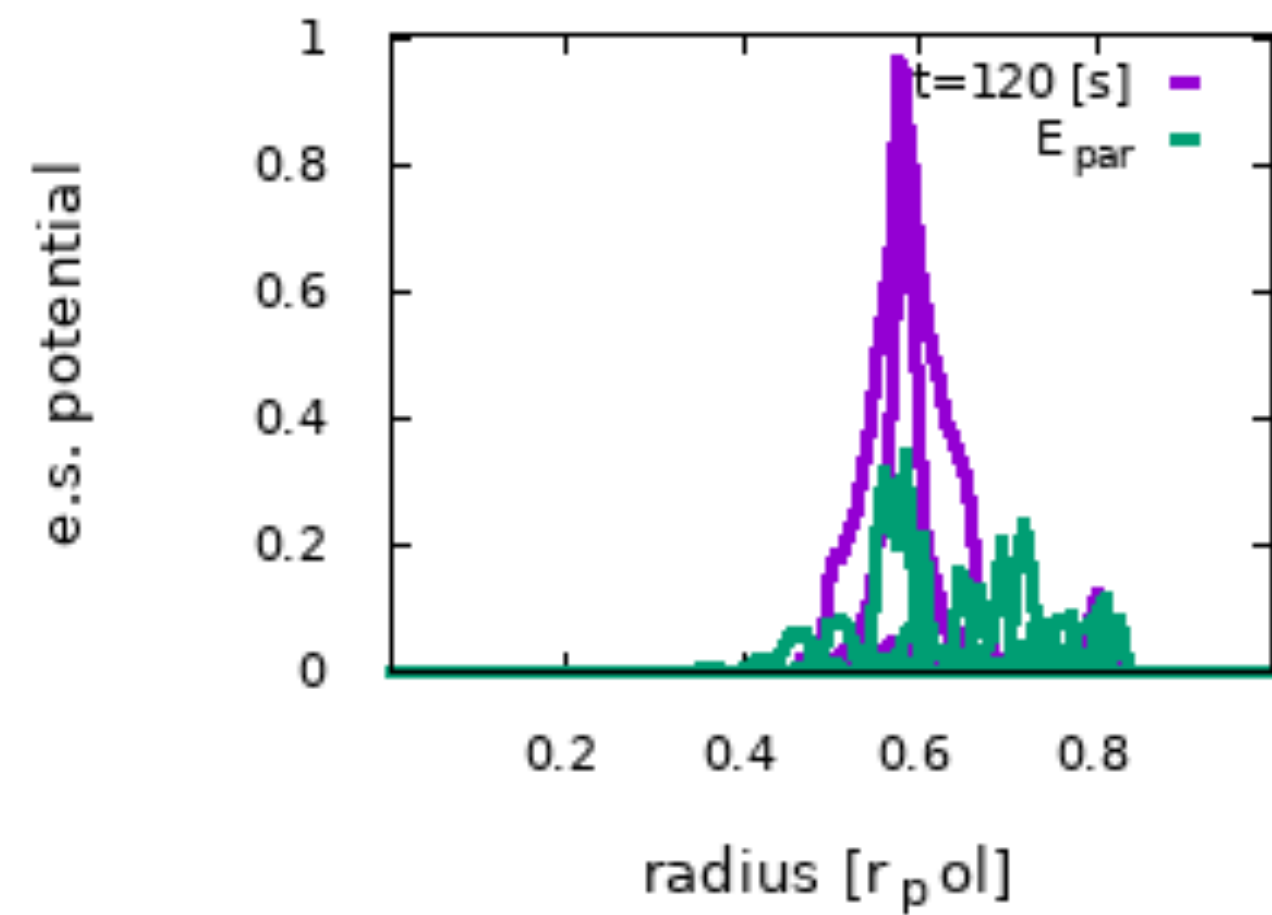
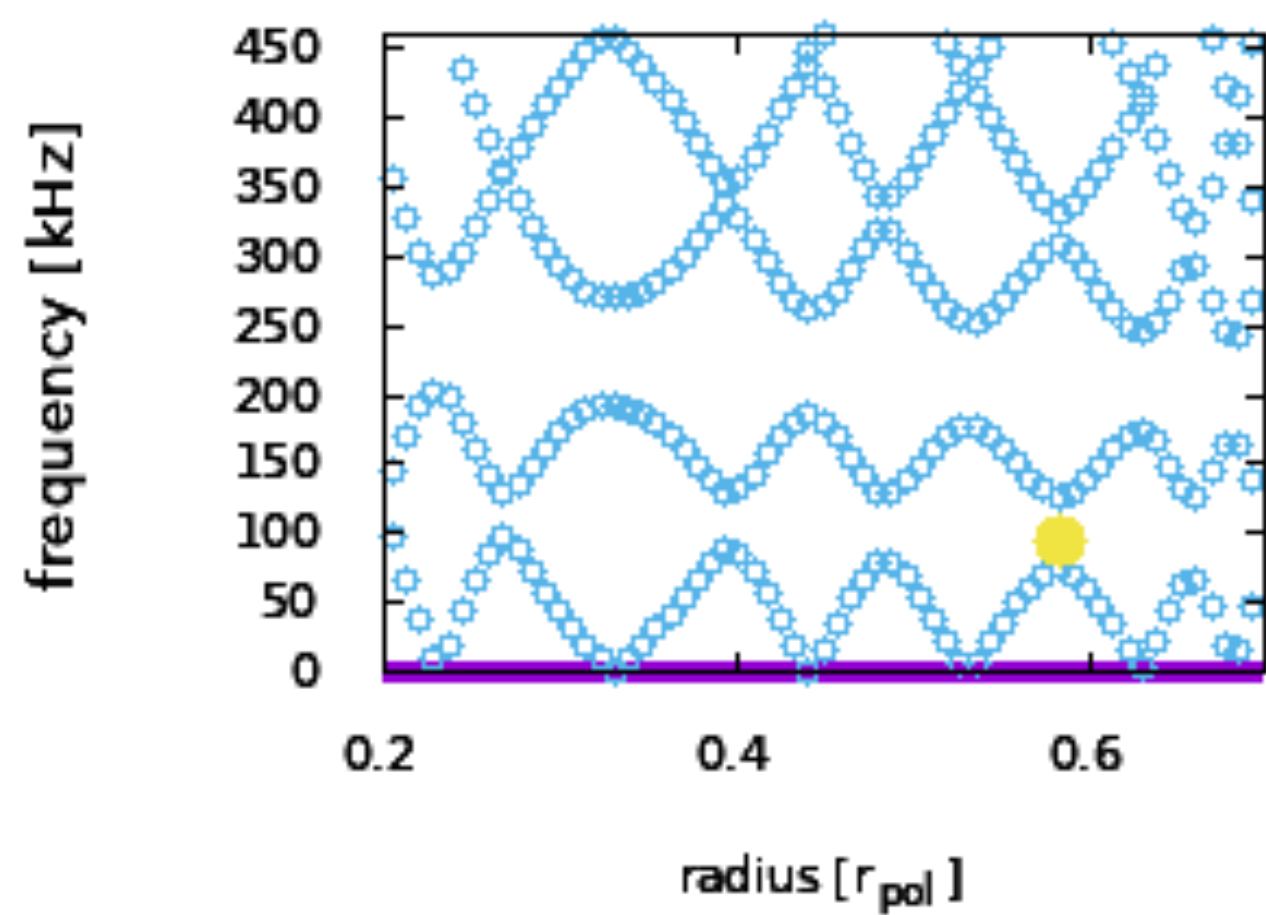
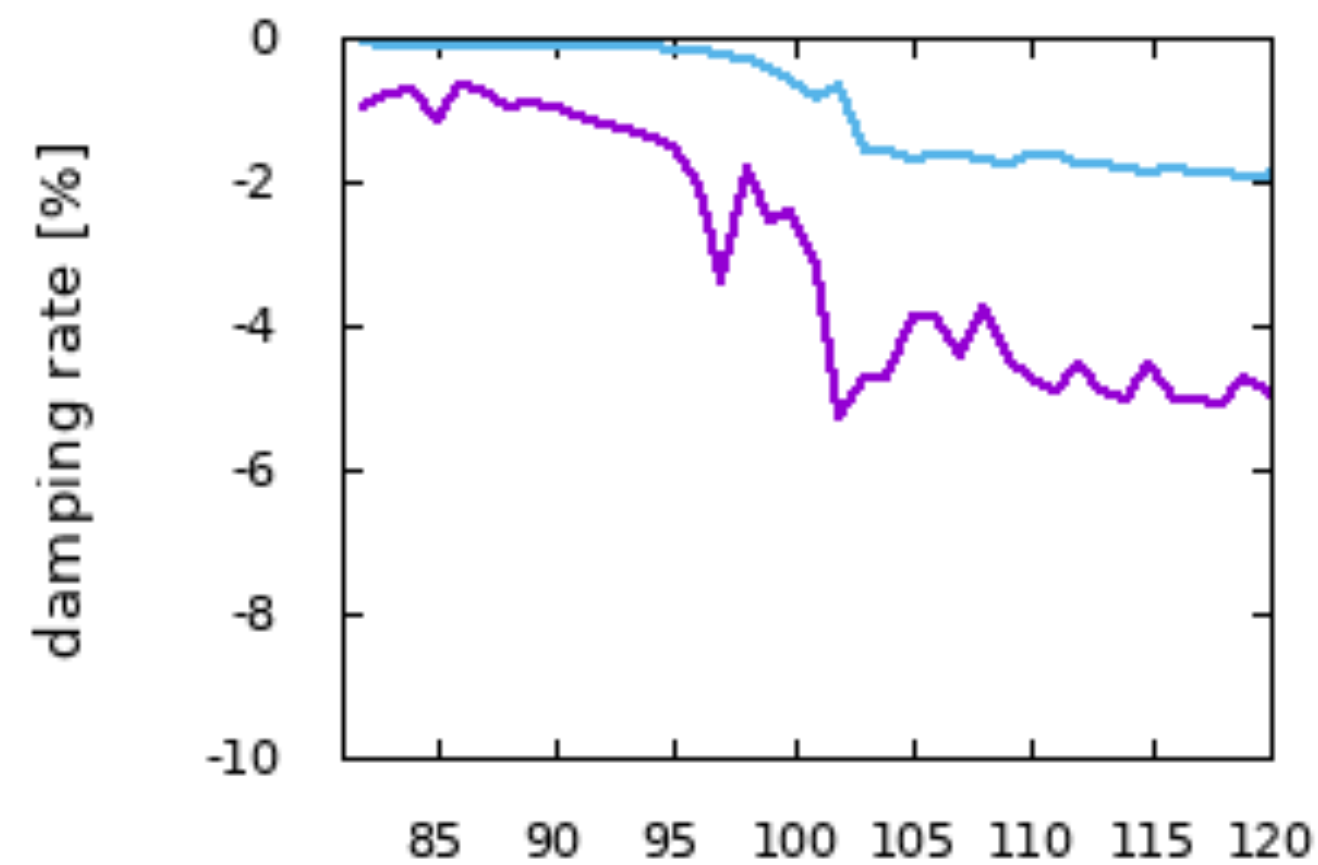
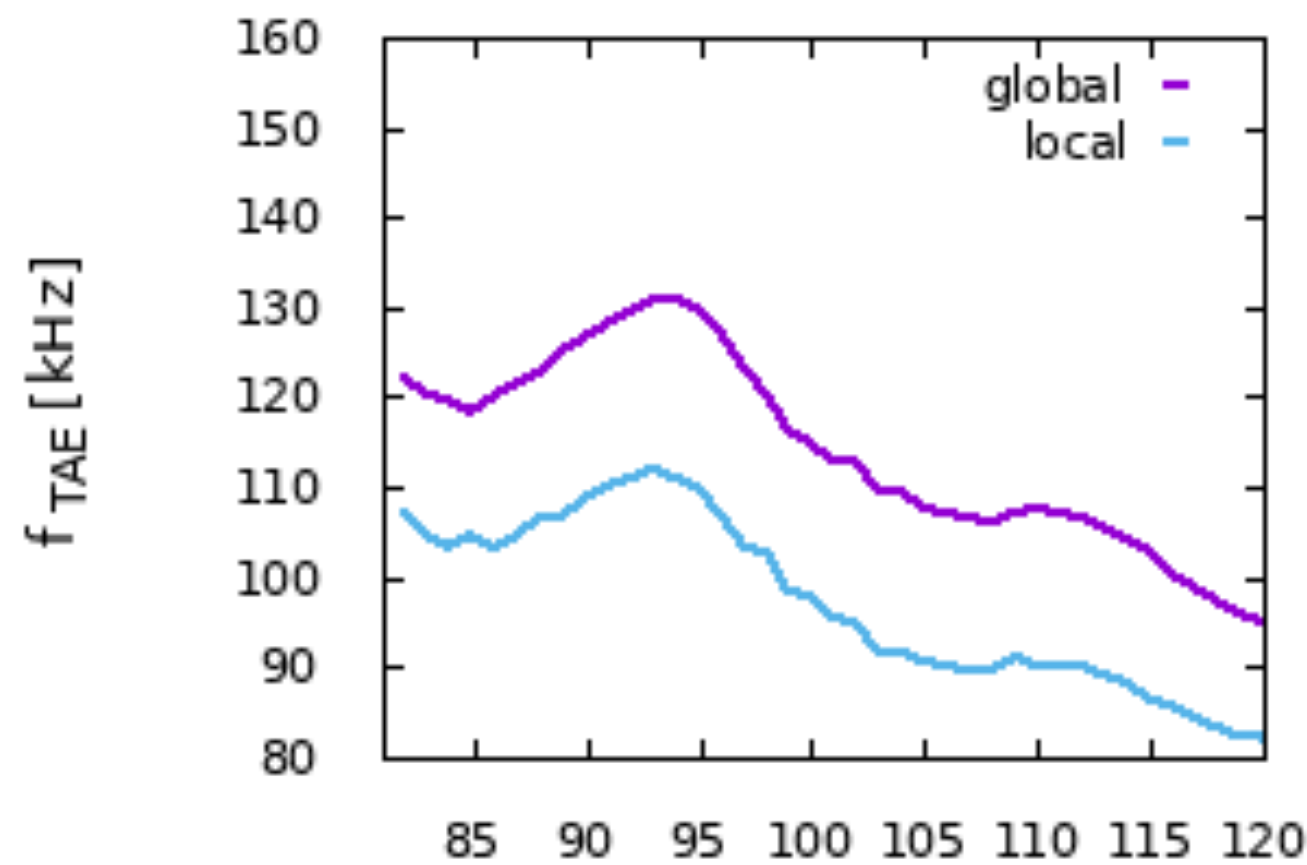


TAE n=12



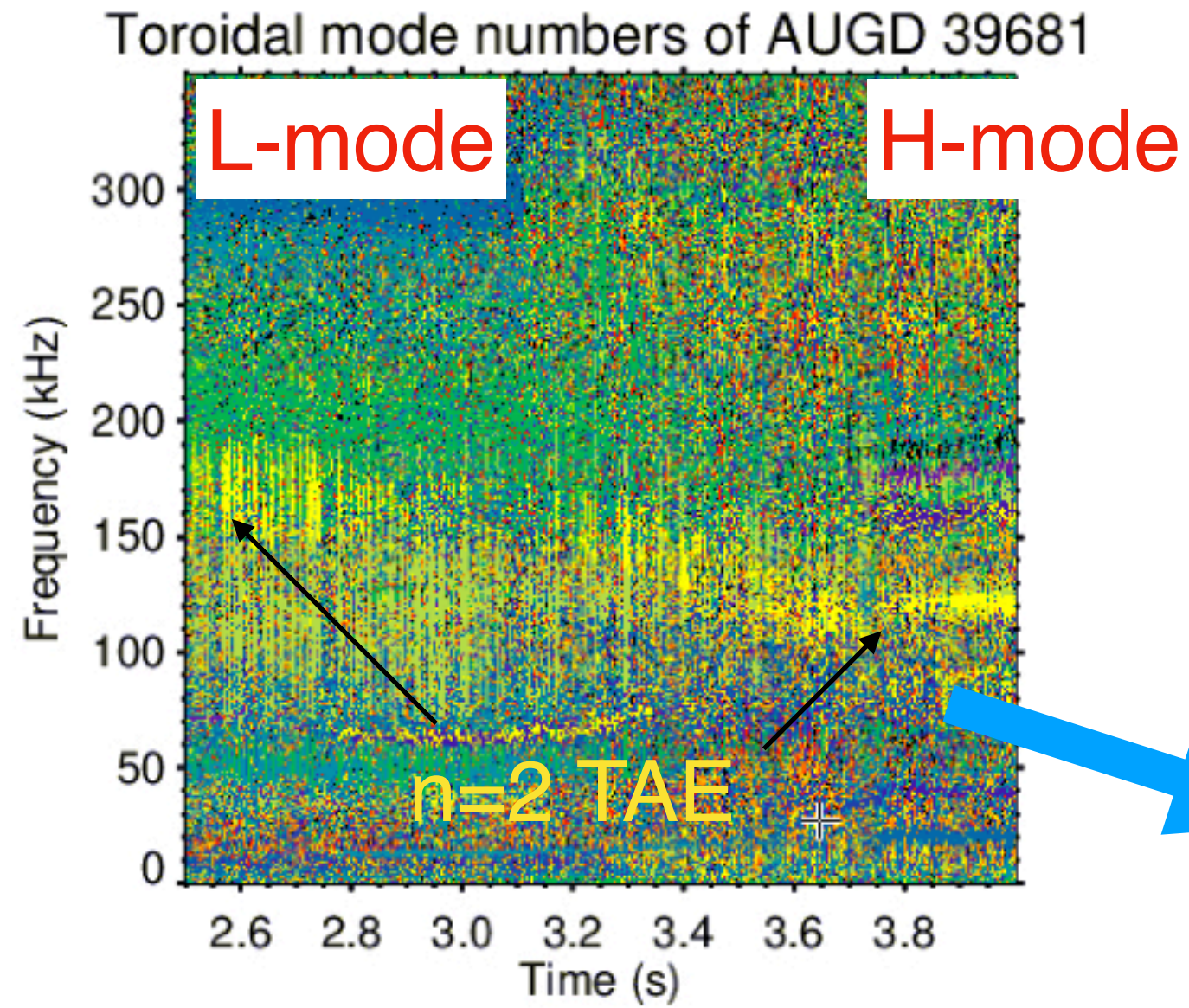
low damping rates during/at the end of the power ramp-up phase

TAE n=18



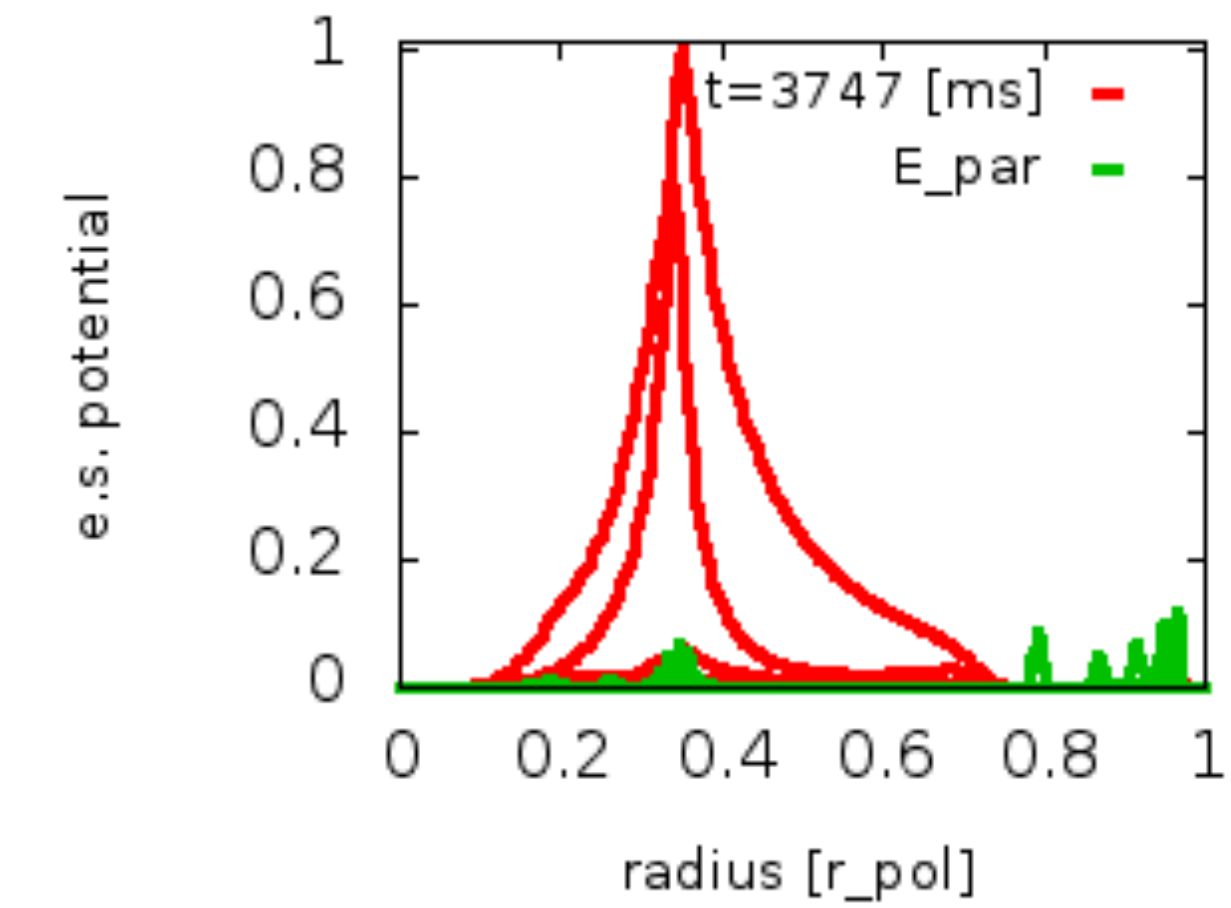
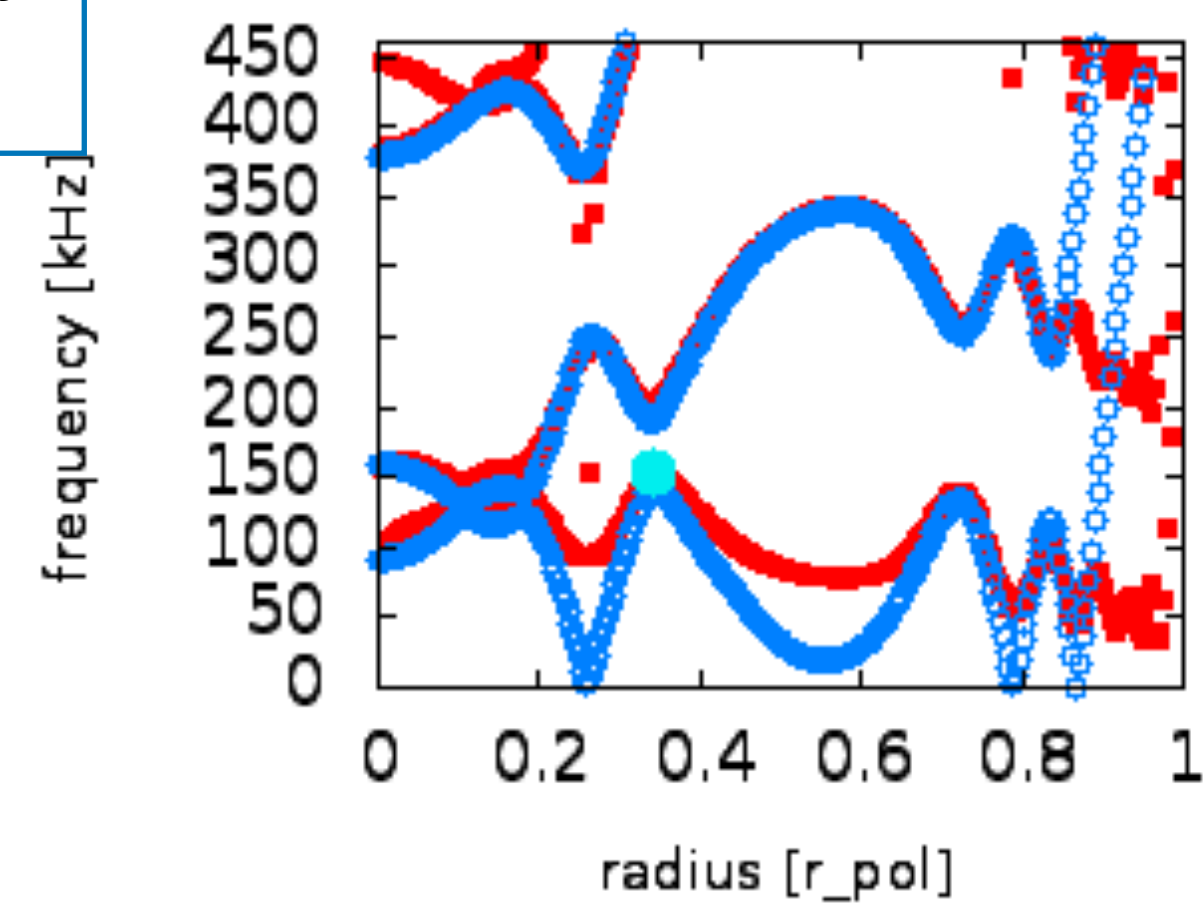
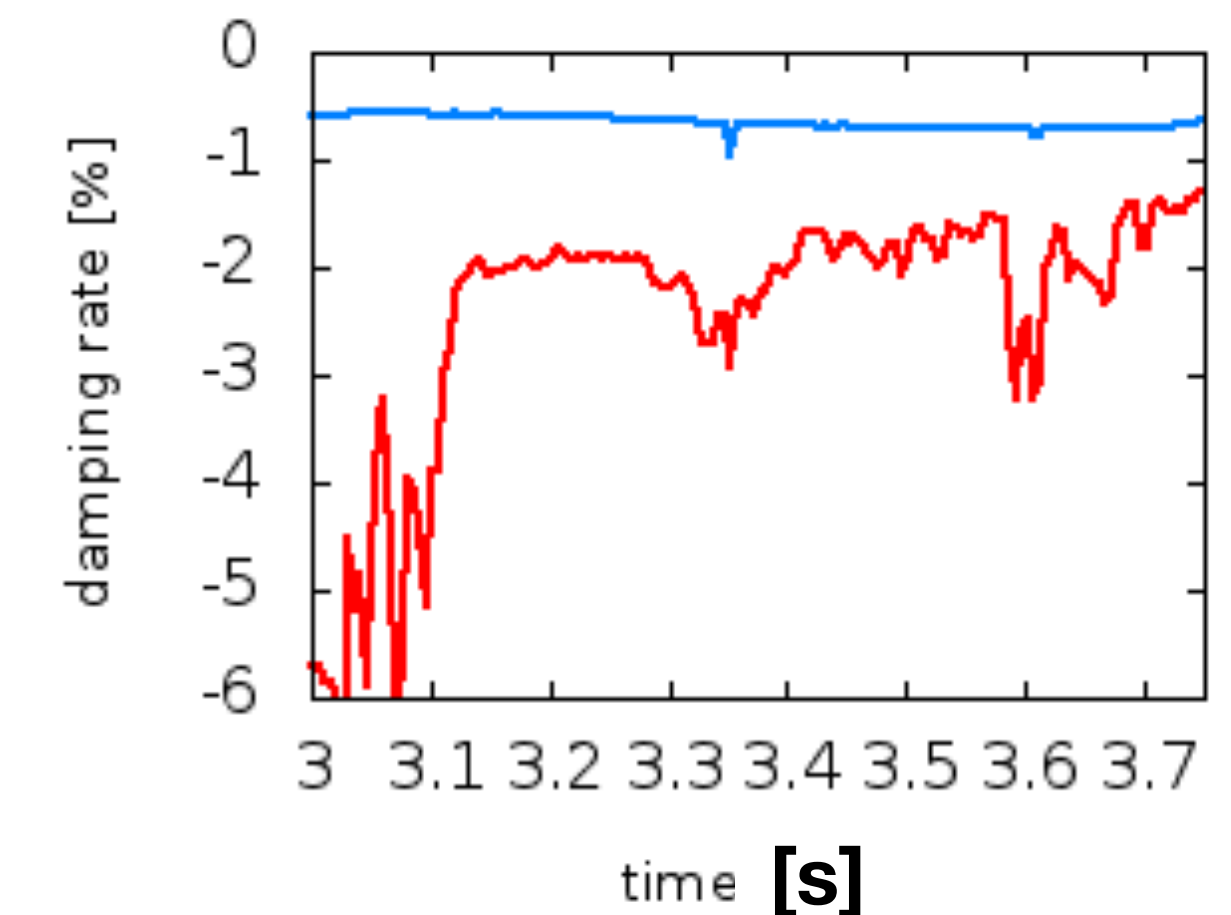
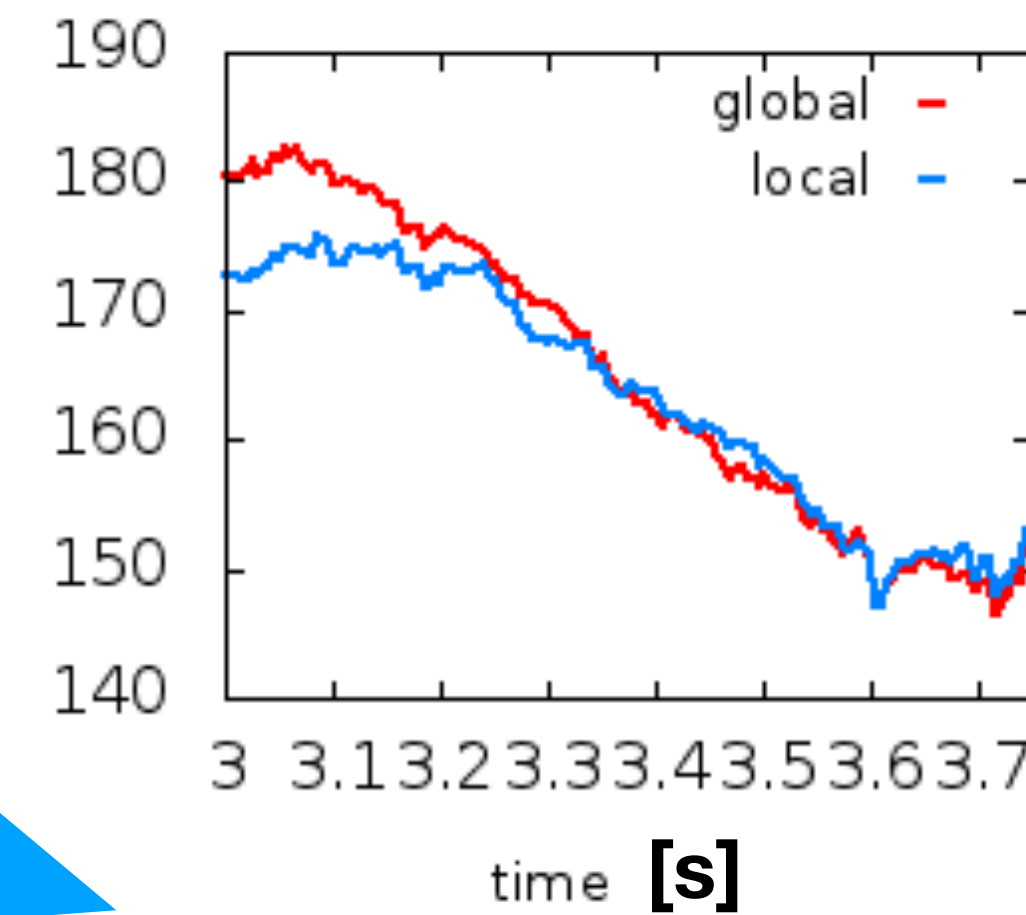
low damping rates during/at the end of the power ramp-up phase

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

integrated data analysis
+
TRVIEW(IMAS interface)
+
EP-WF: LIGKA local
+
EP-WF: LIGKA global

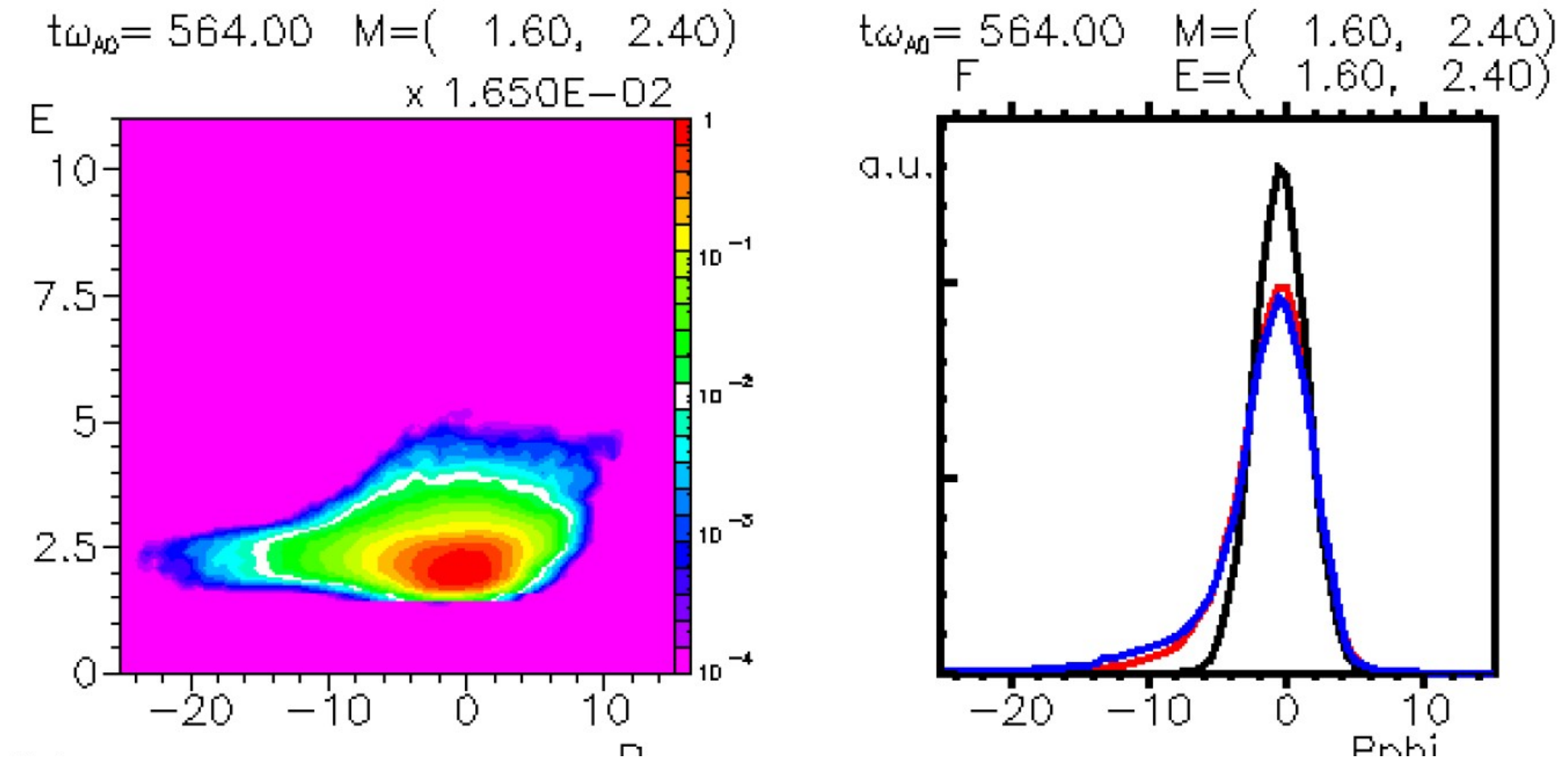


- analyse L-mode, H-mode and transition phase using
- also systematic uncertainty quantification feasible

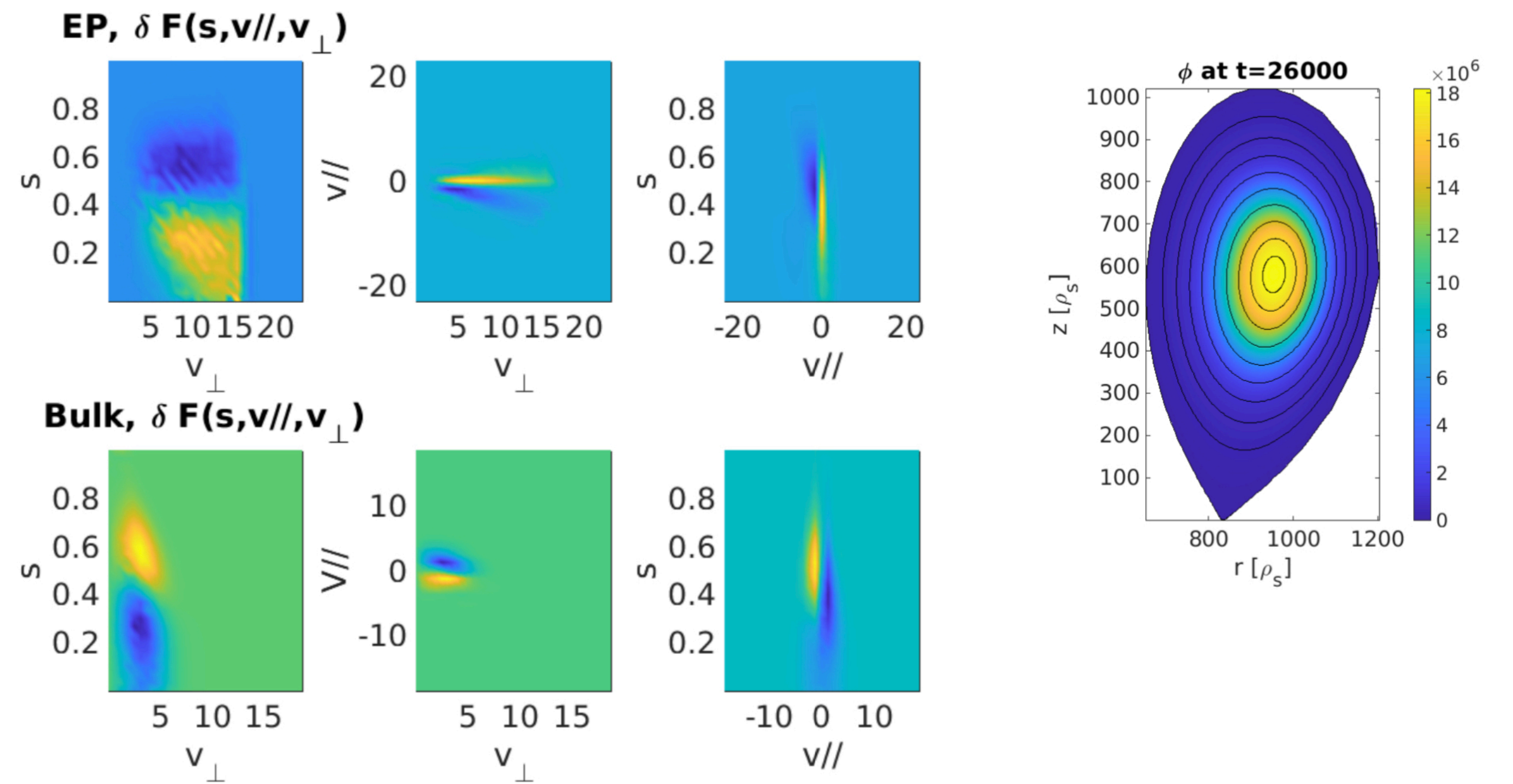


calculating PSZSs

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, Varenna 2022]

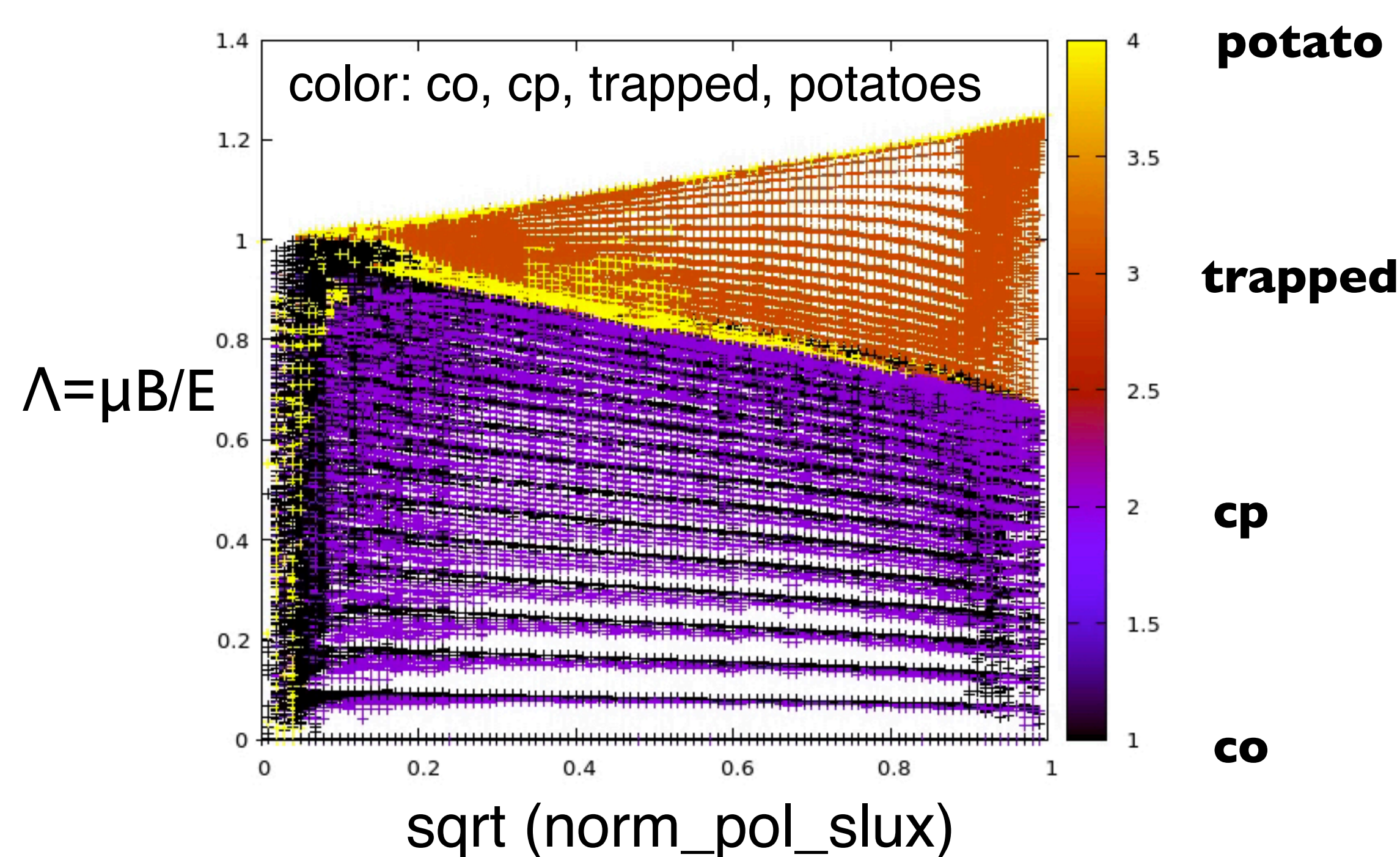
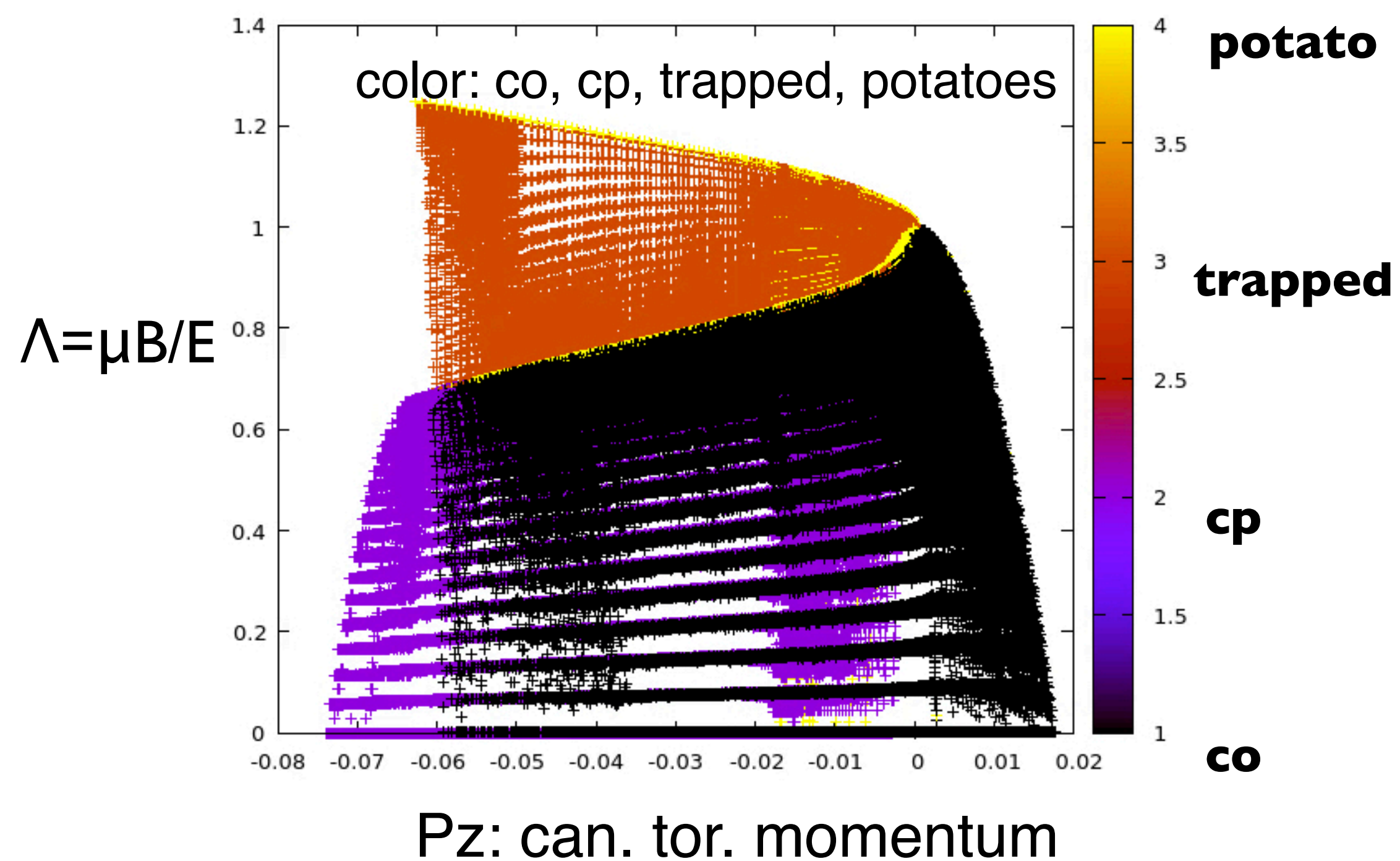


calculating PSZSs based on orbit/zonal averaging



- use IMAS-based wrapper program for HAGIS to set up marker space, determine trapped-passing boundary, sort, classify, orbit averages for unperturbed equilibria
- originally developed to calculate propagator integrals for LIGKA

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



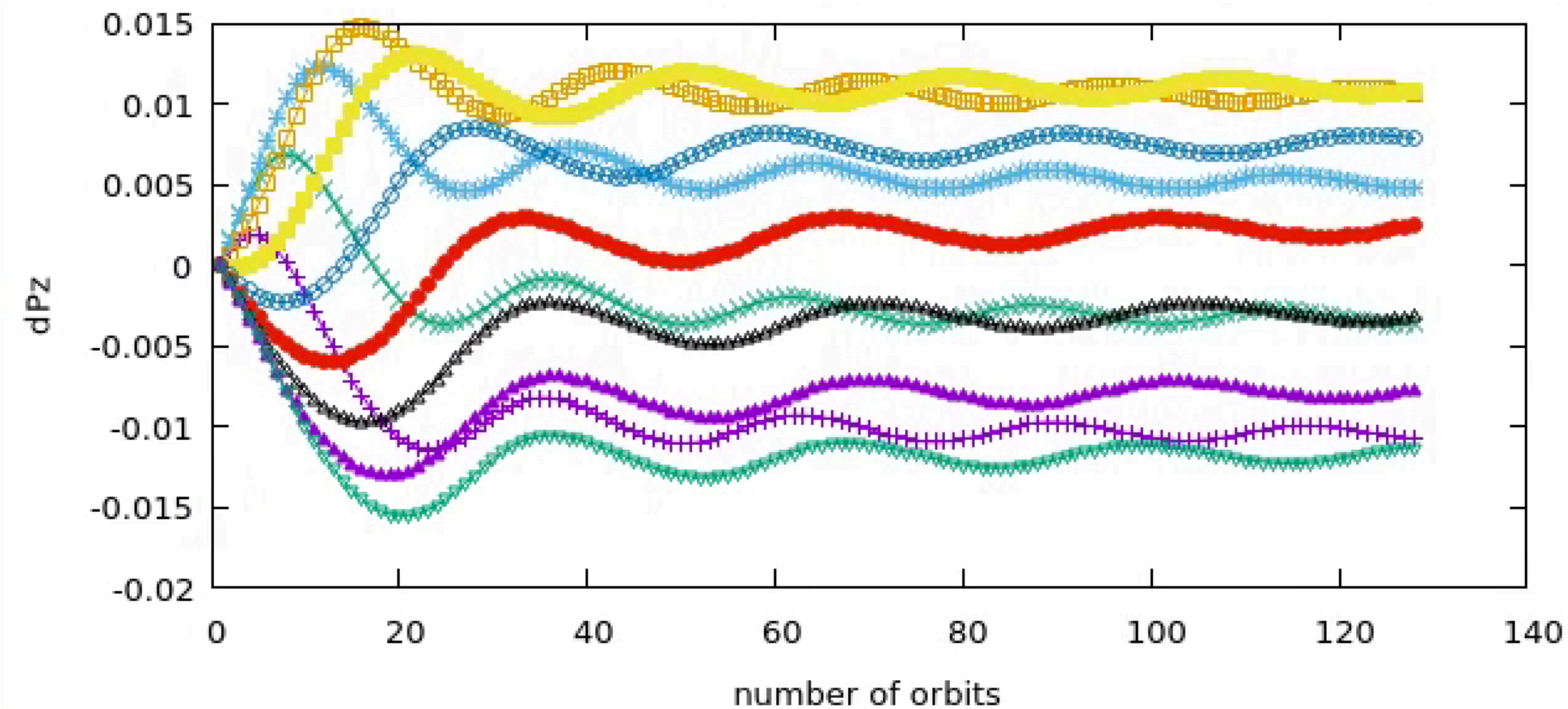
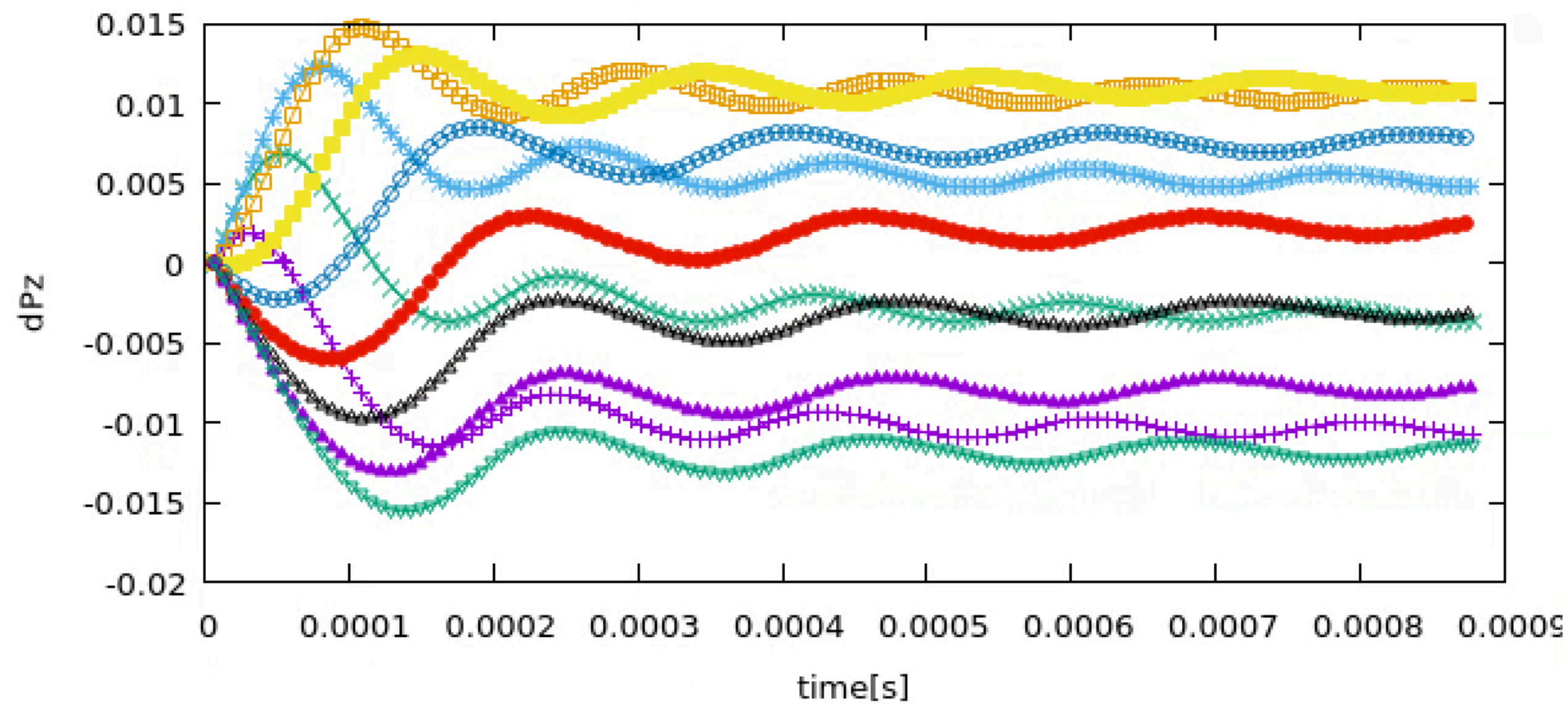
- distributions IDS holds all orbit-averaged information about marker space
- fast, repetitive calls of HAGIS library within IMAS are possible - **mapping between Pz and <radial position>!**

calculating PSZS using HAGIS



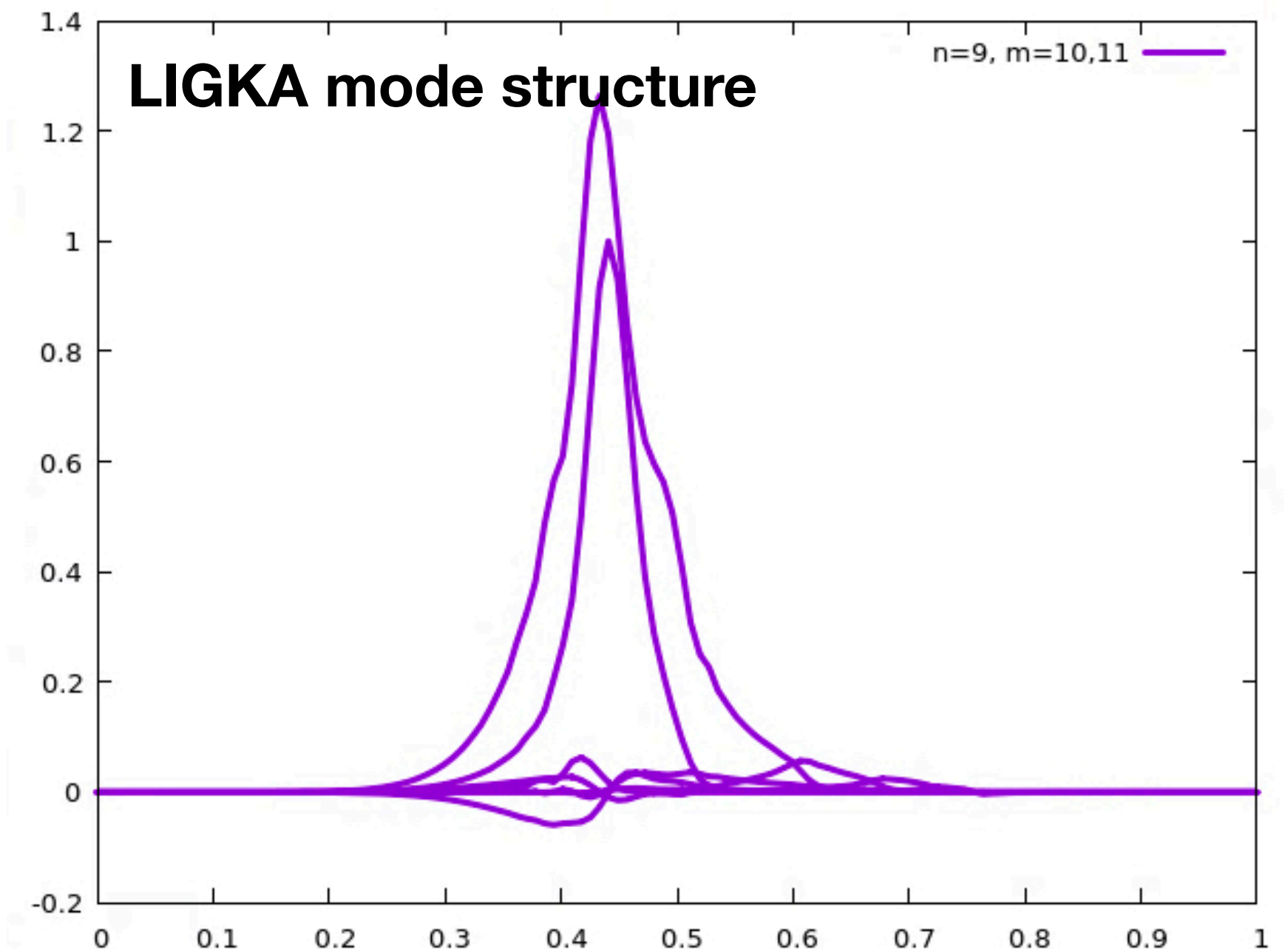
adding LIGKA calculated perturbation: follow set of markers for wave-periods, time or number of orbits

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

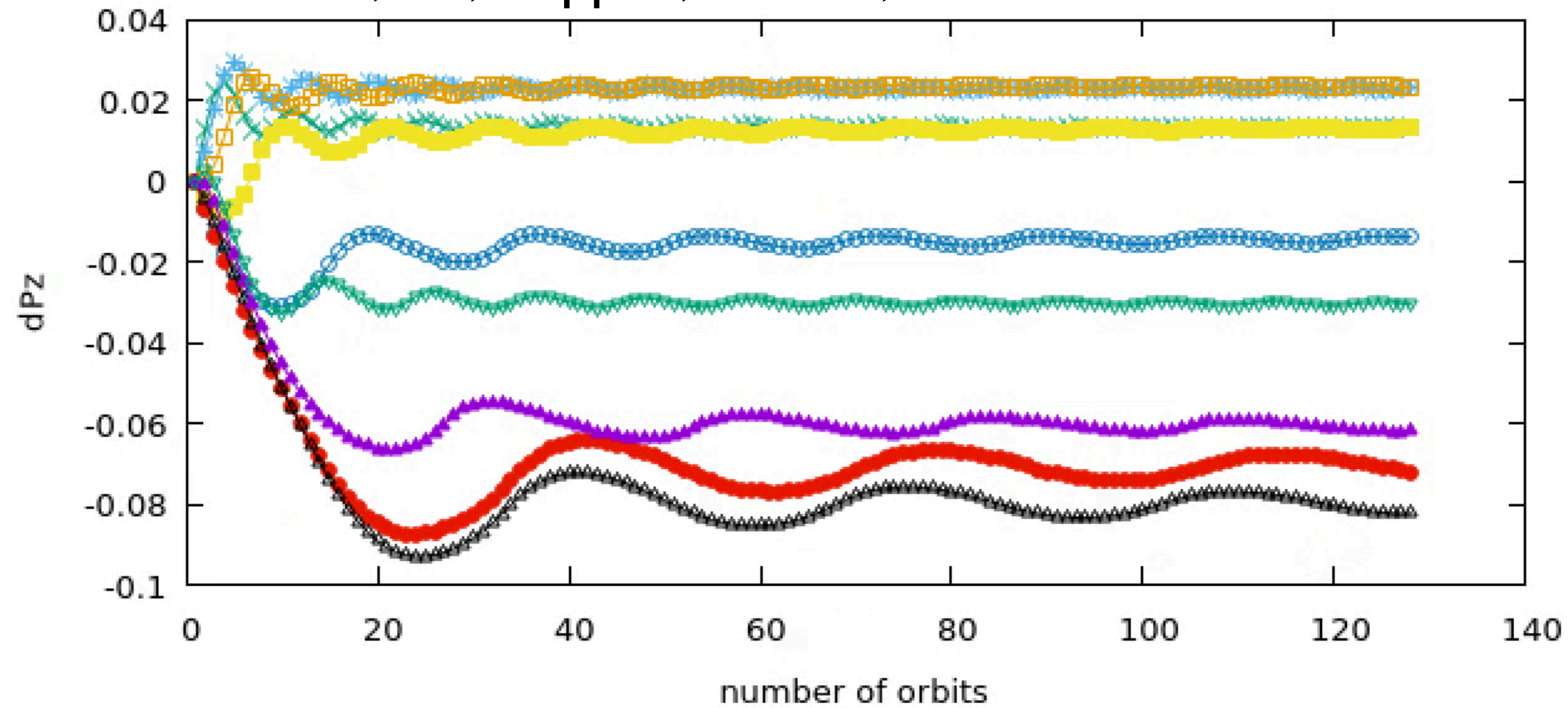


colours: different starting phase, 10 markers with starting tor. angle $[0: 2\pi/n]$

important: averaging over phase is crucial to obtain correct fluxes

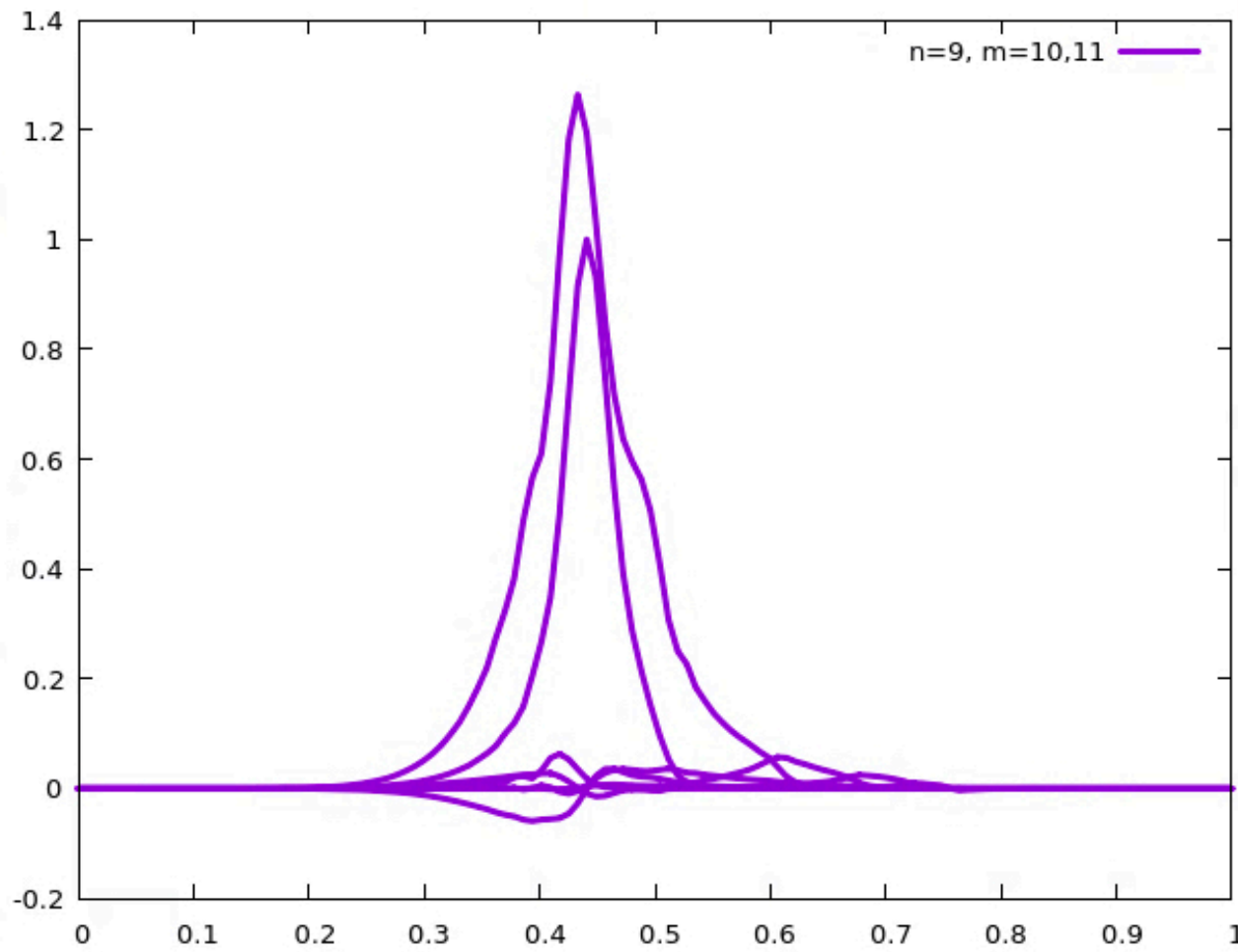


1 MeV, He, trapped, $\Lambda=1.03$, $n=9$ TAE with $dB/B=10^{-3}$

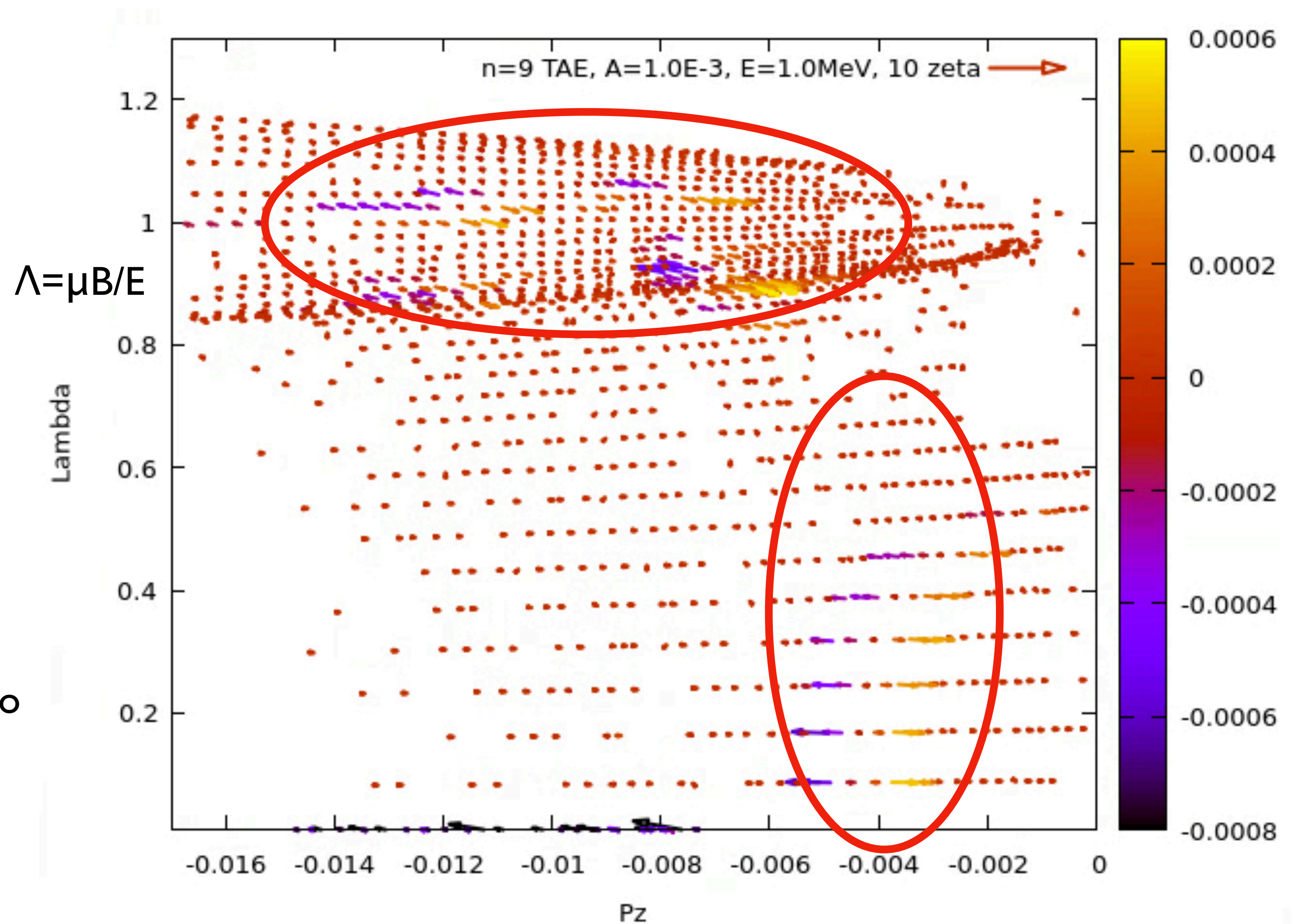


averaging over markers with different phase gives effective poloidally and toroidally averaged dPz

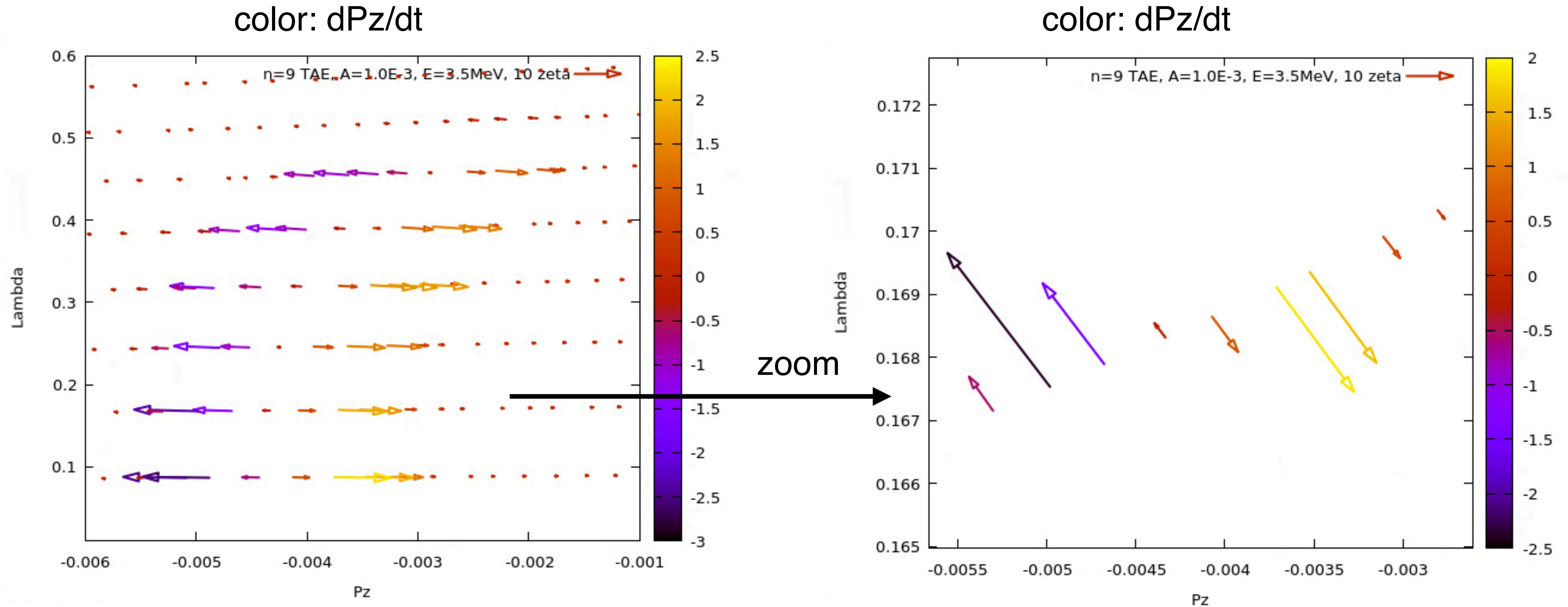
what is dP_z , dE , $d\Lambda$ for given perturbation after x completed orbits?



- arrows: initial $(P_z, \Lambda) \rightarrow (P_z + \delta P_z, \Lambda + \delta \Lambda)$
- color: δP_z
- averages over 10 phases, 10 orbits
- 3-5 minutes to calculate
- modular structure of wrapper code allows to replace HAGIS with newer/faster code of same functionality

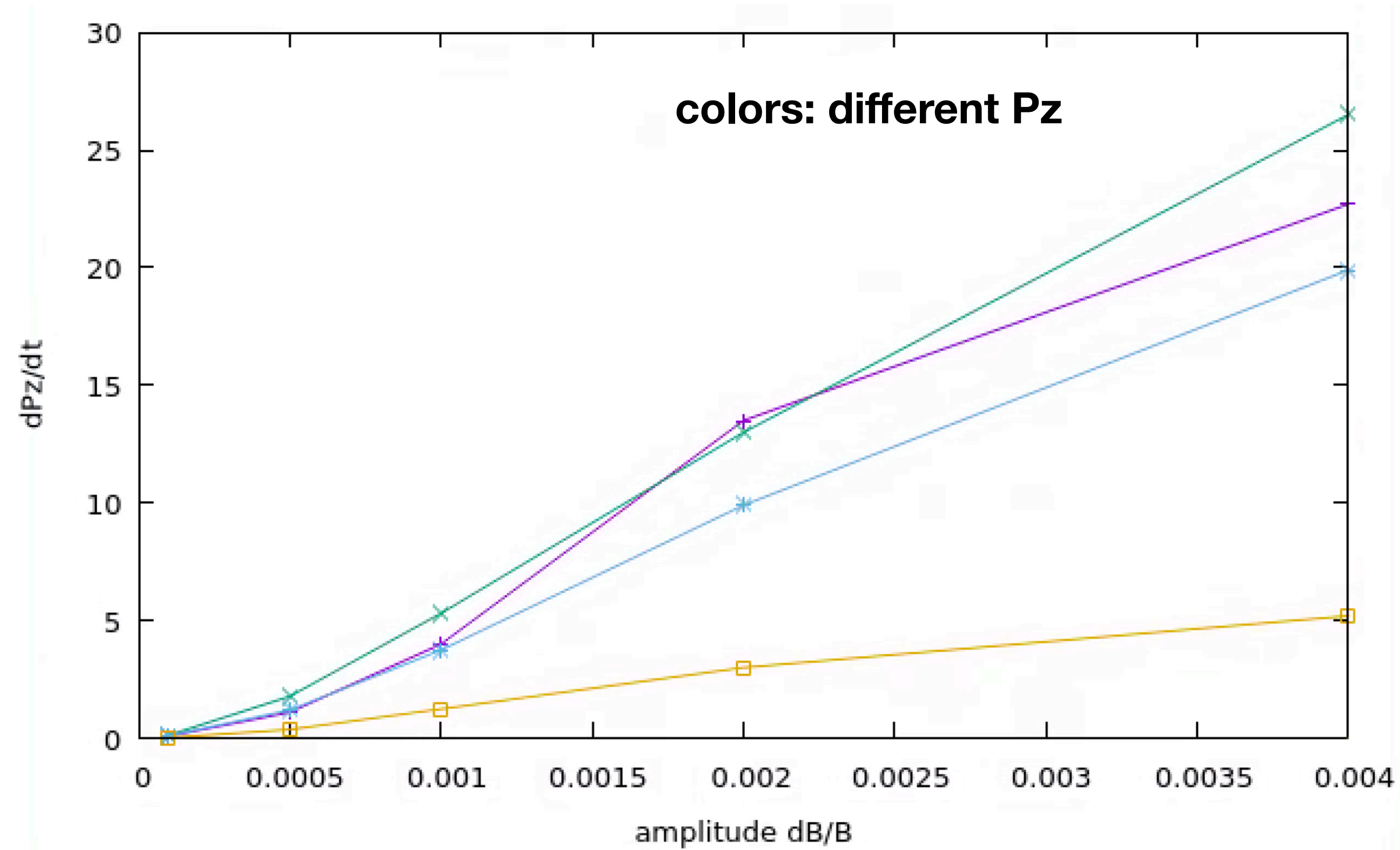


calculate fluxes: dP_z/dt [(eV/s)/s]



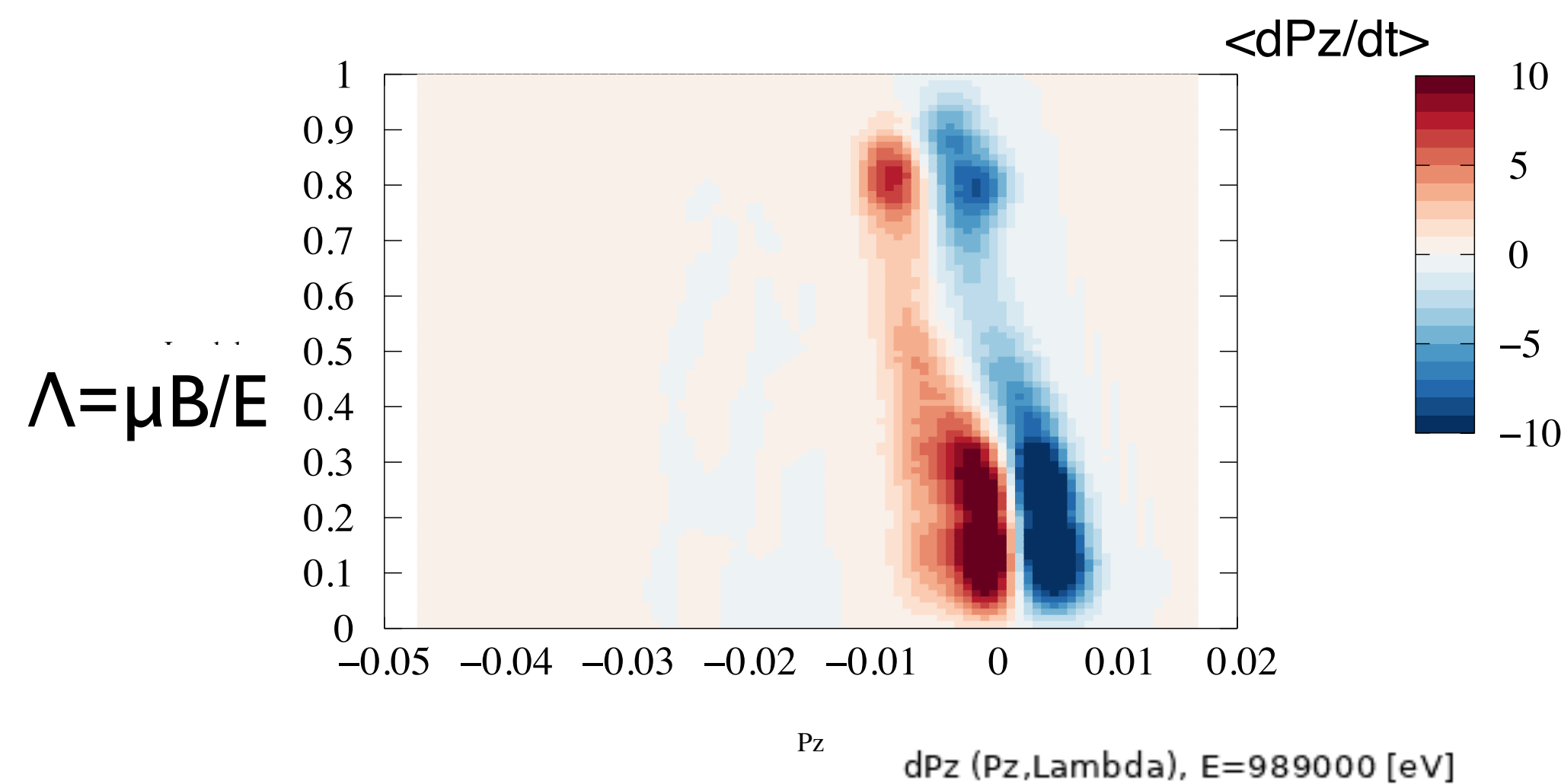
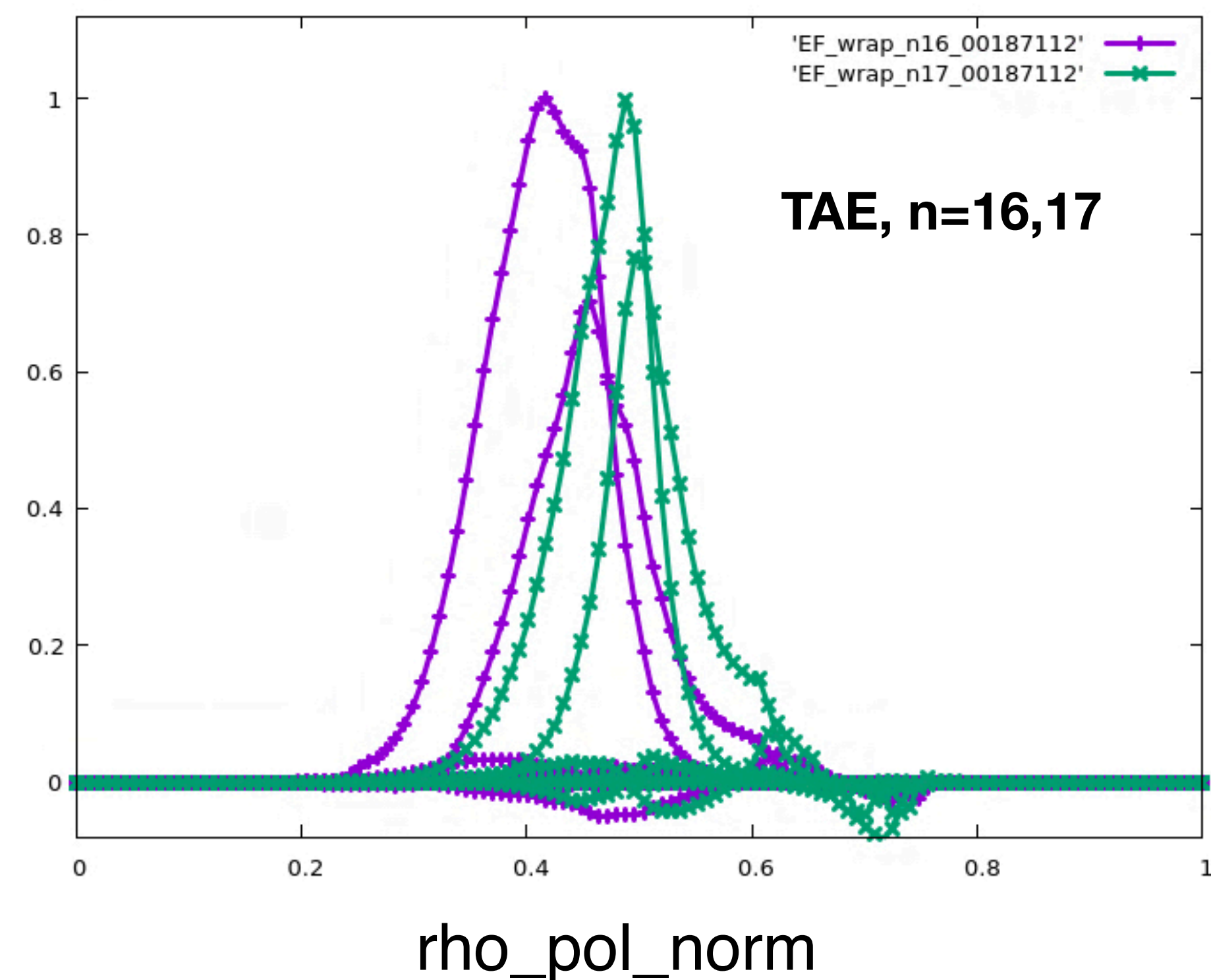
- divide δP_z by orbit transit time and number of orbits (here 32)
- the same information is available for Λ and E
- transport coefficients $D_{P_z}=(dP_z)^2/dt$ and $K_{P_z}=(dP_z)/dt$ can be evaluated

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

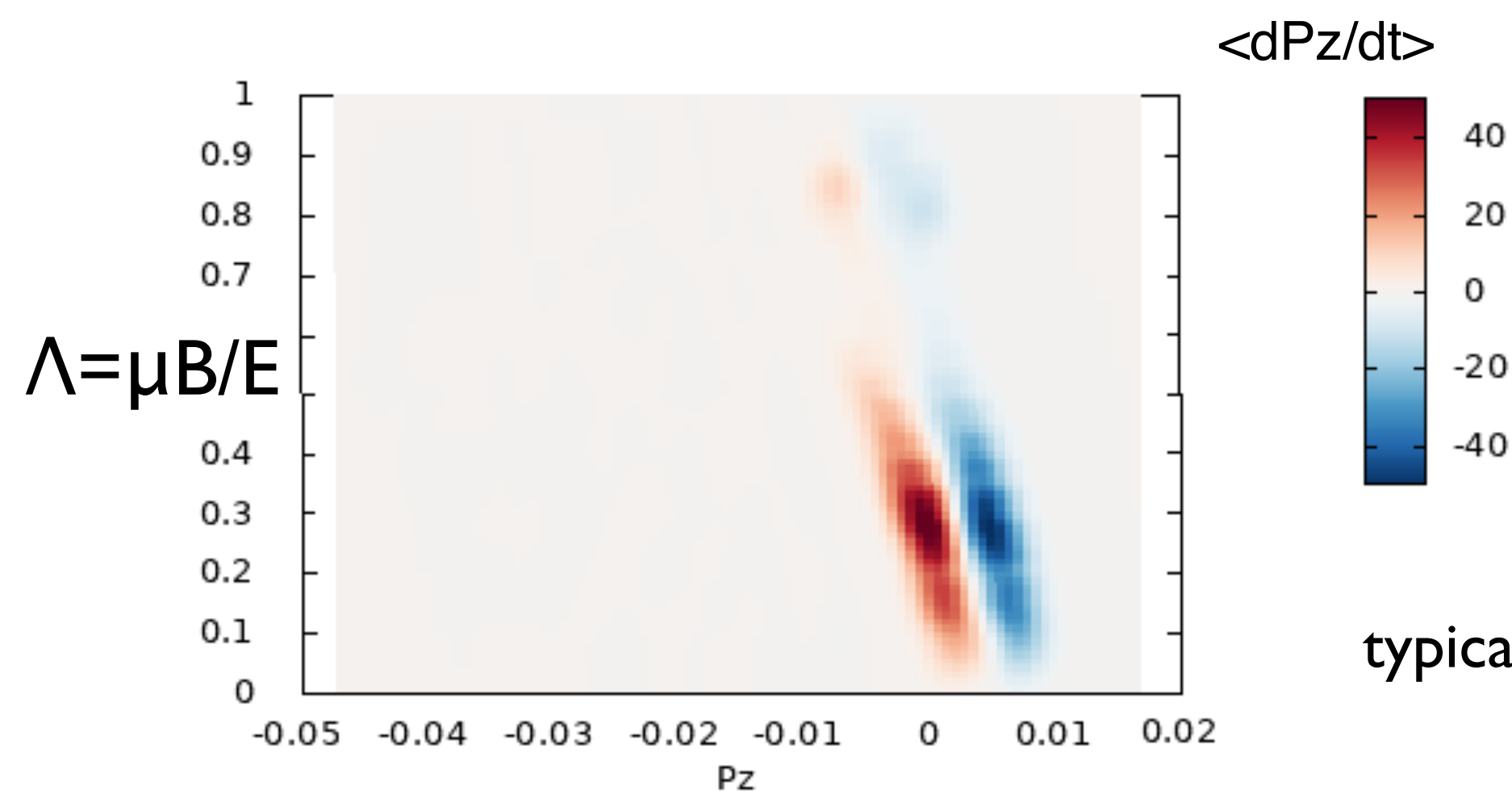


- dPz/dt as function of perturbation size: simple interpolation captures the amplitude scaling

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



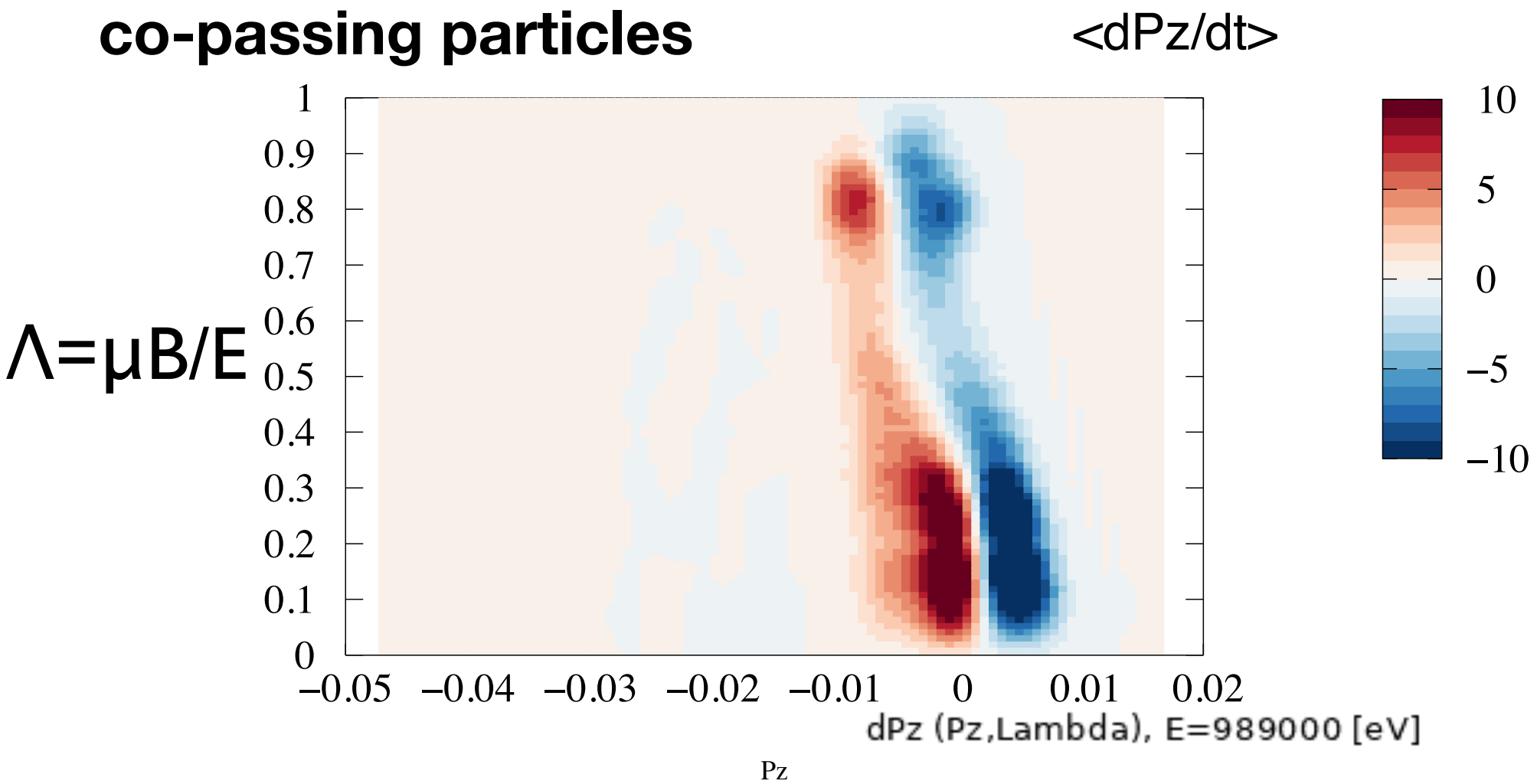
co-passing particles,
energy averaged



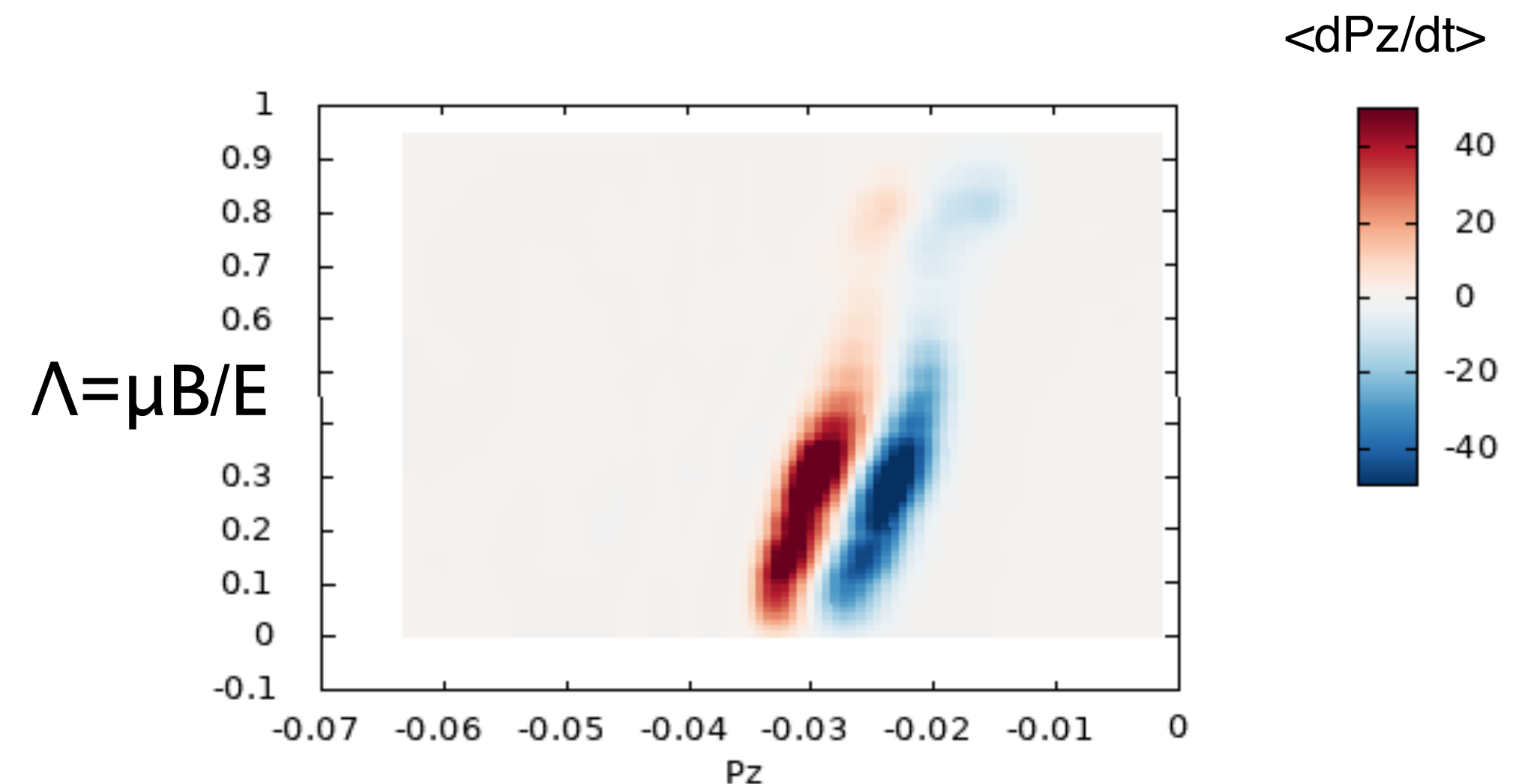
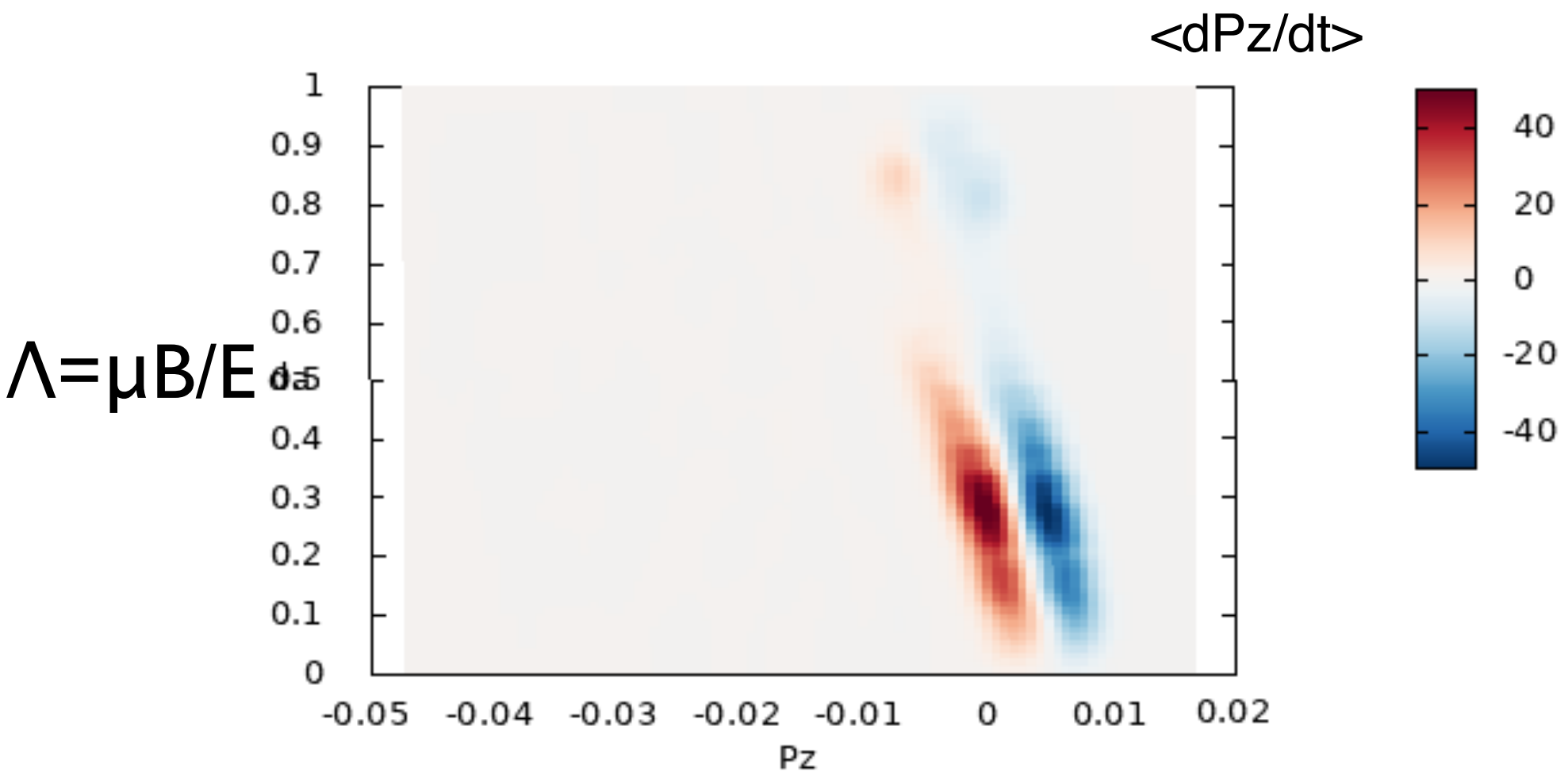
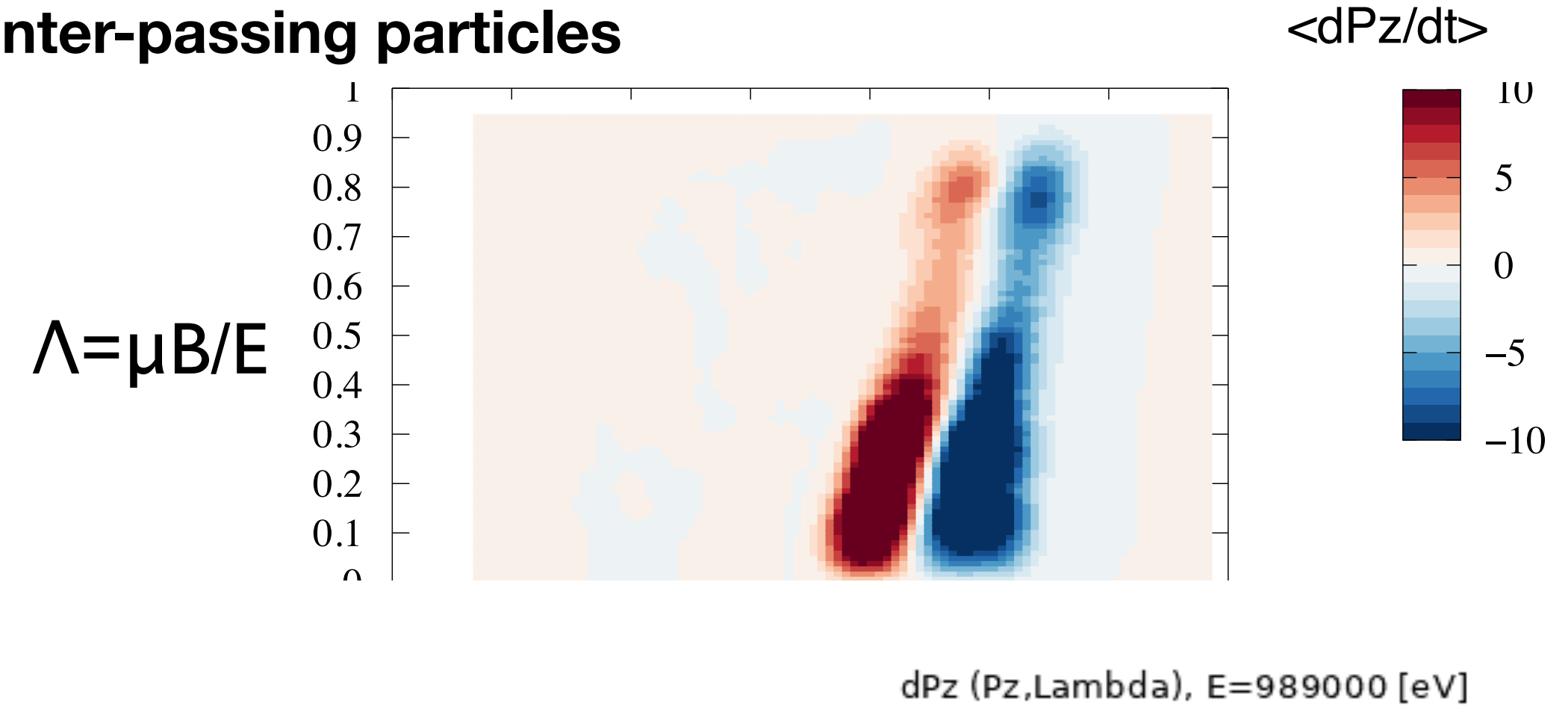
typical grid: (P_z, E, Λ) (128x40x40)

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co-passing particles

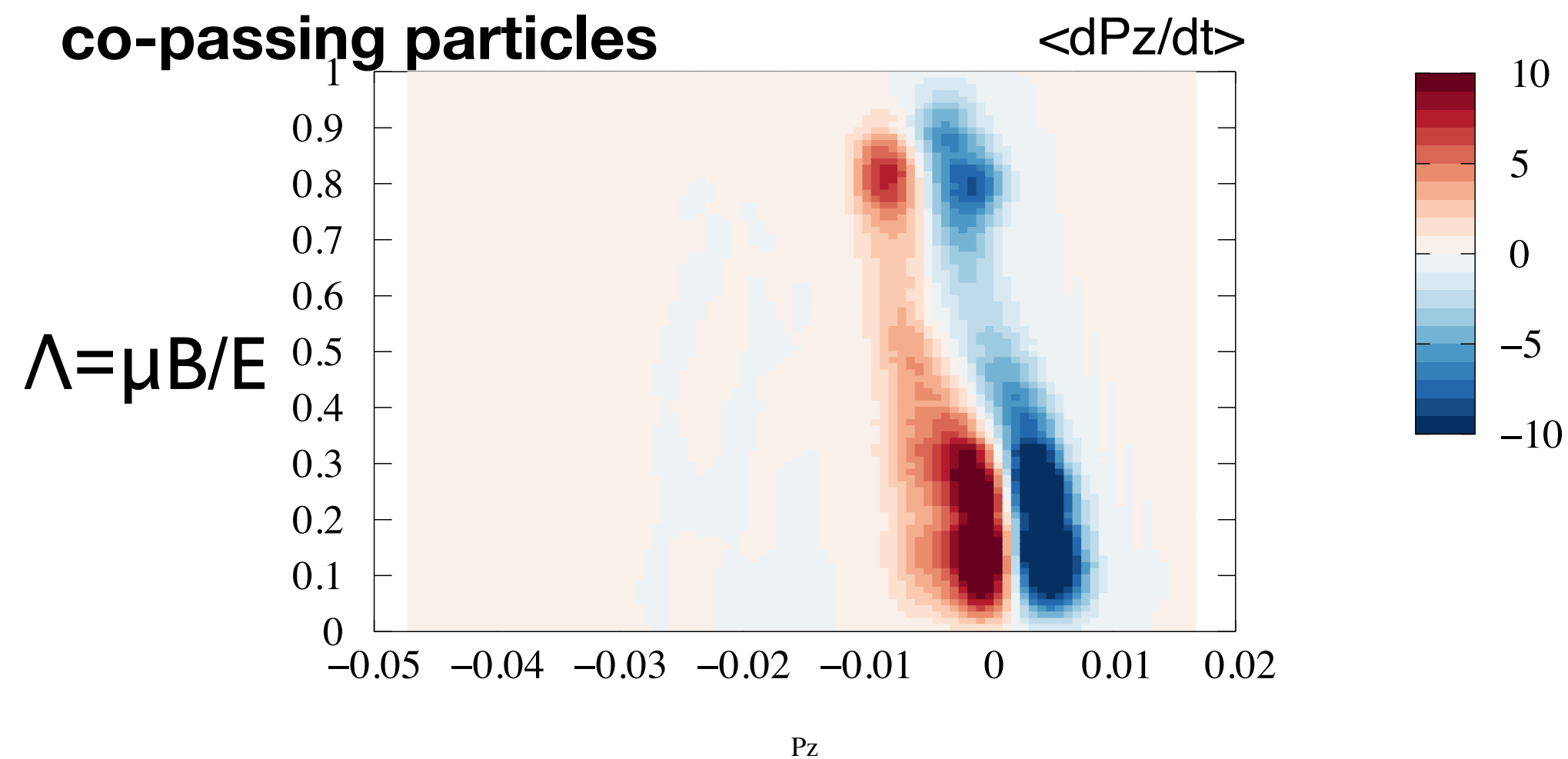


counter-passing particles

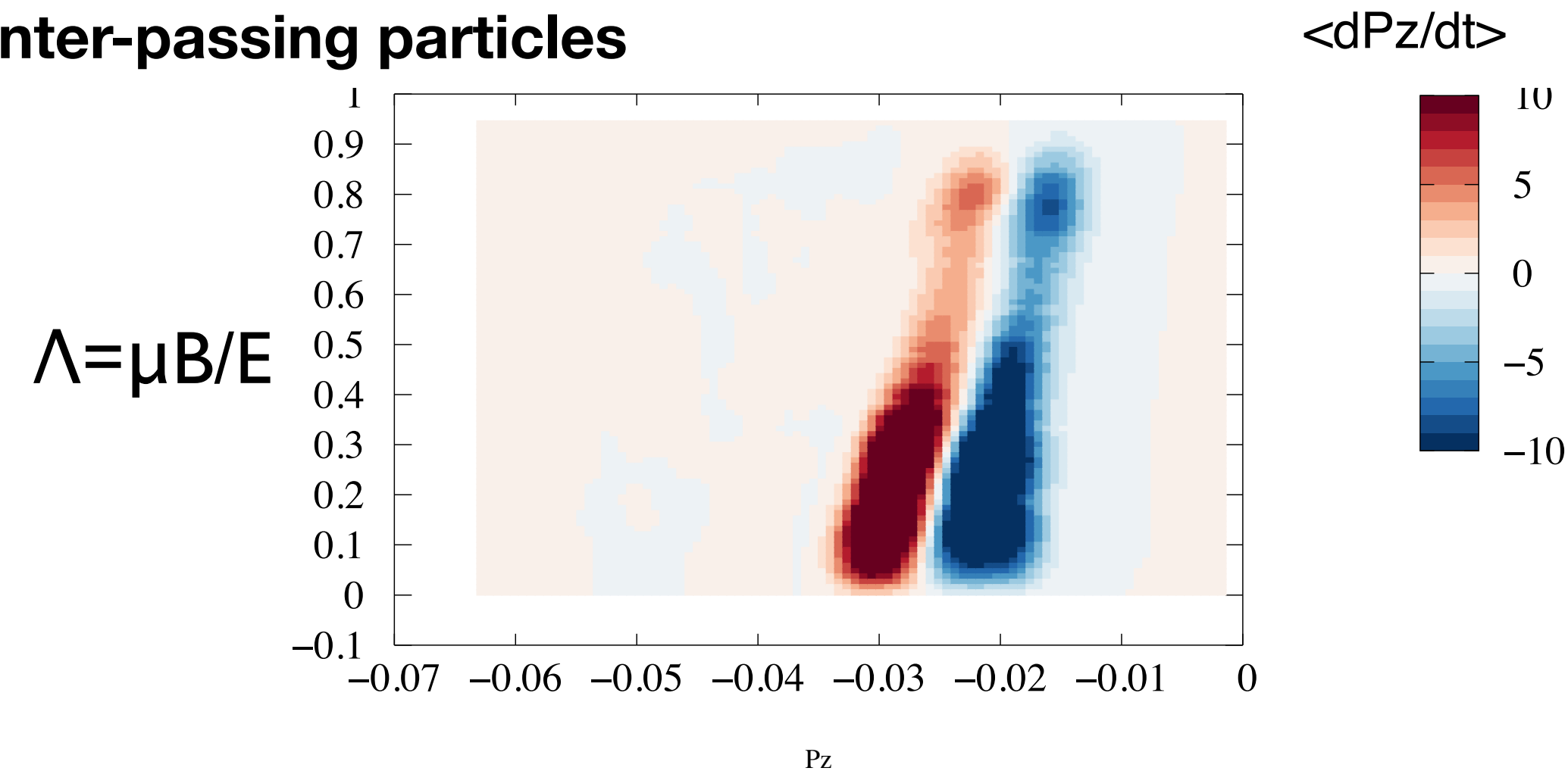


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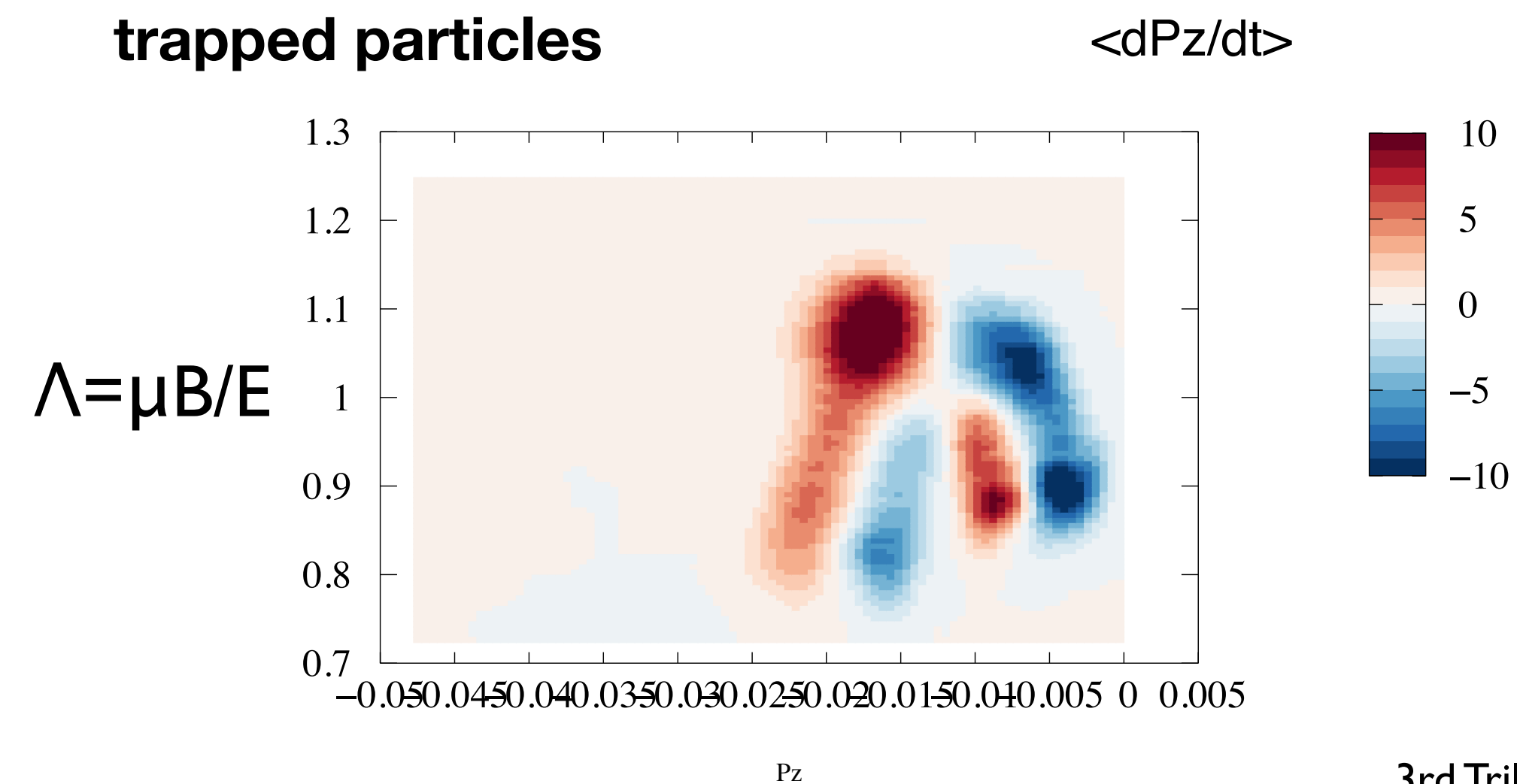
co-passing particles



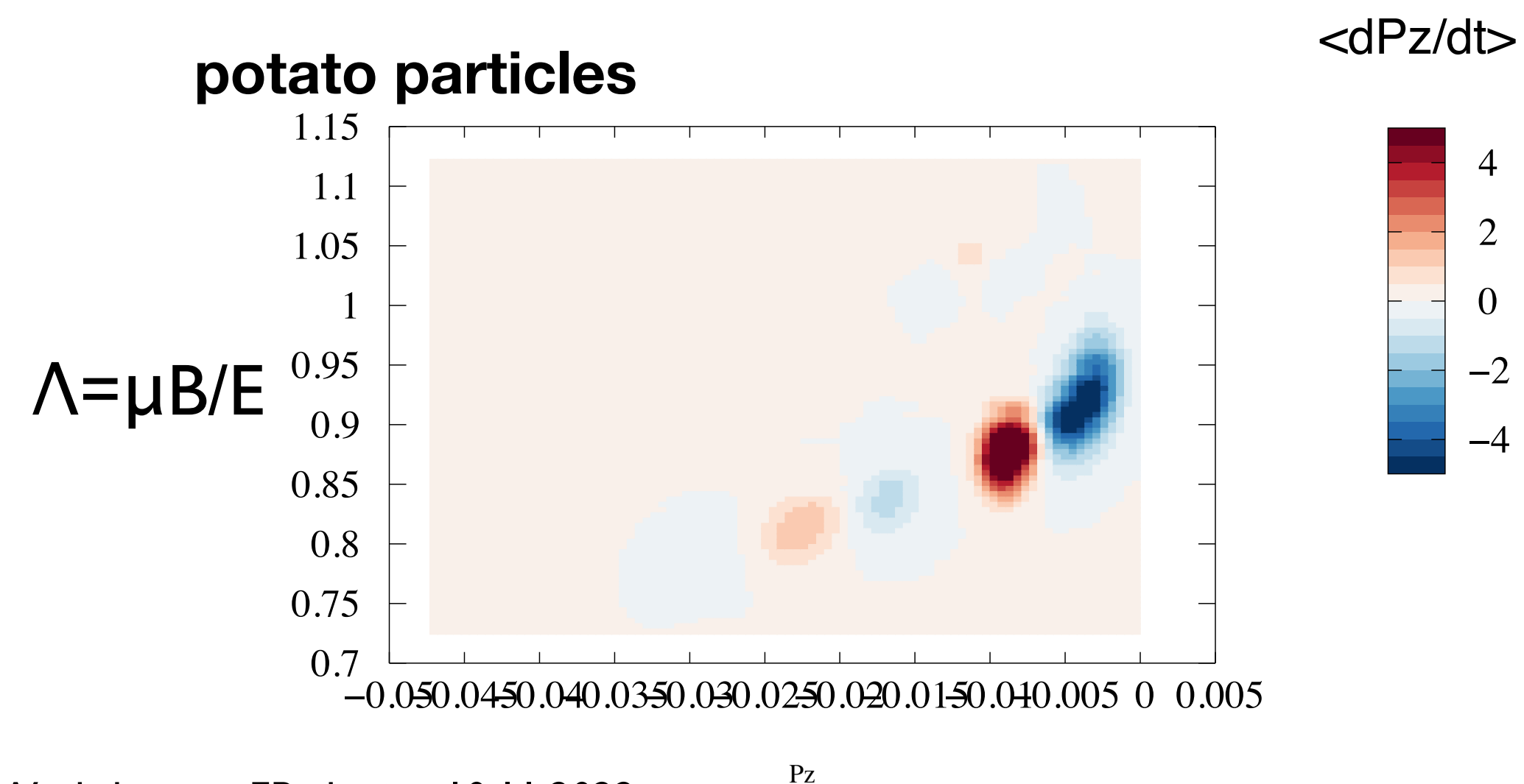
counter-passing particles



trapped particles

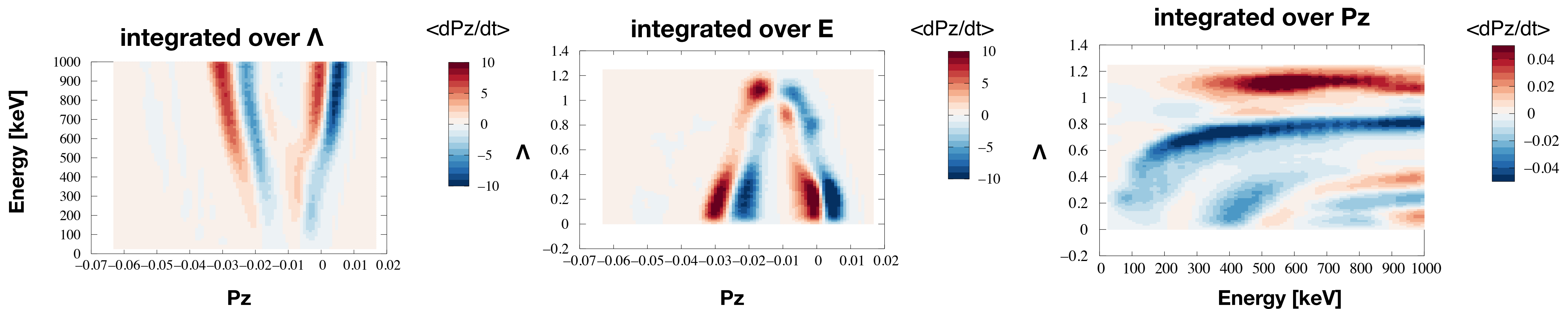


potato particles

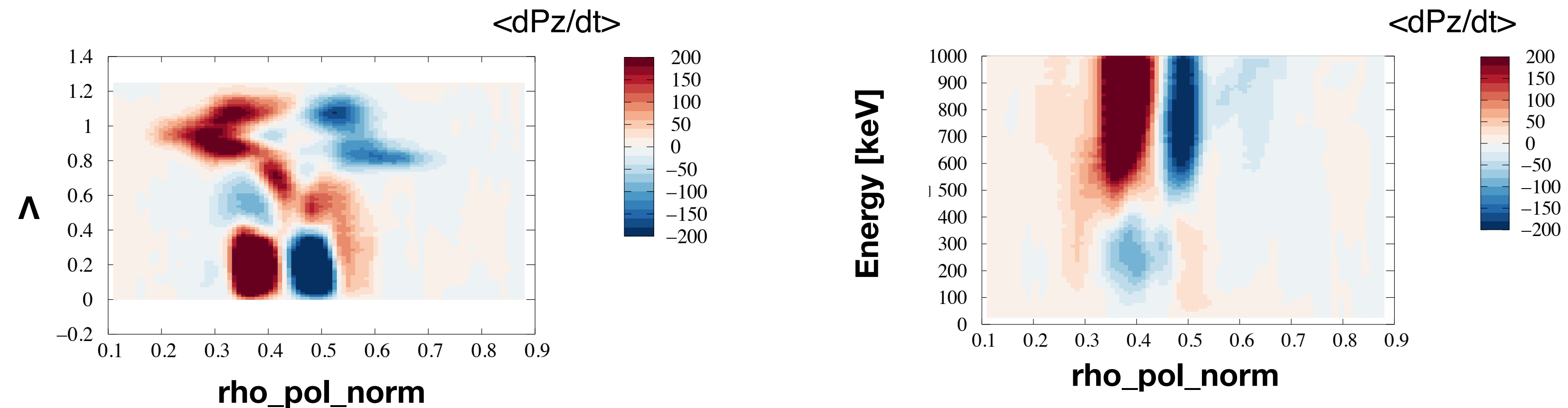


- calculate $\langle dP_z/dt \rangle$, $\langle dE/dt \rangle$ for given fixed mode structures at fixed amplitude with FINDER/HAGIS, write into IDS
- ATEP code: read PSZS data, use 3D bspline methods to create $\langle dP_z/dt \rangle$, $\langle dE/dt \rangle$ on 3D grid as F_{EP}
- use 3d scattered-data b-spline algorithm [Scattered Data Interpolation with Multilevel B-Splines, Lee 1997] - post-smoothing

all particles:

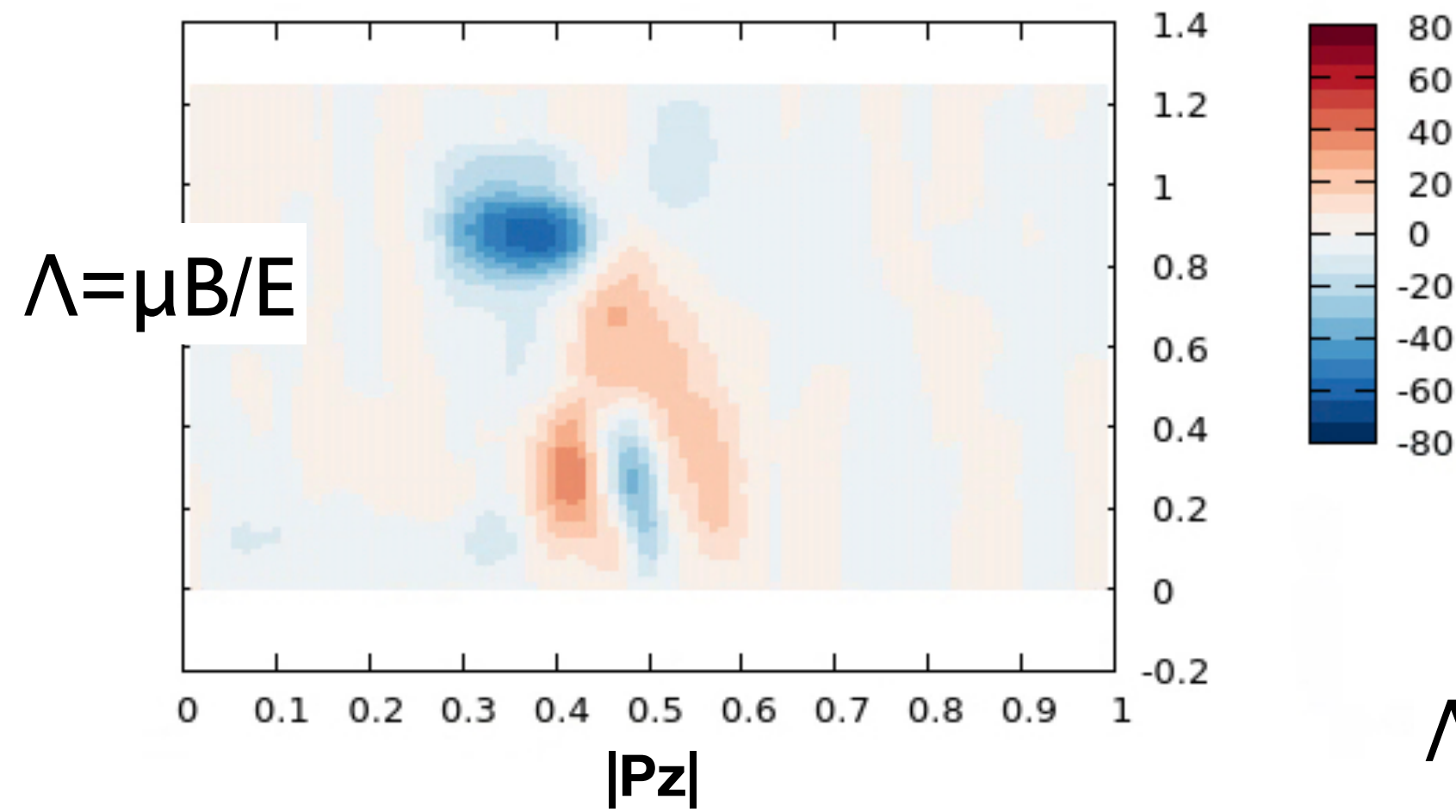


can be easily mapped to $\langle s \rangle$:

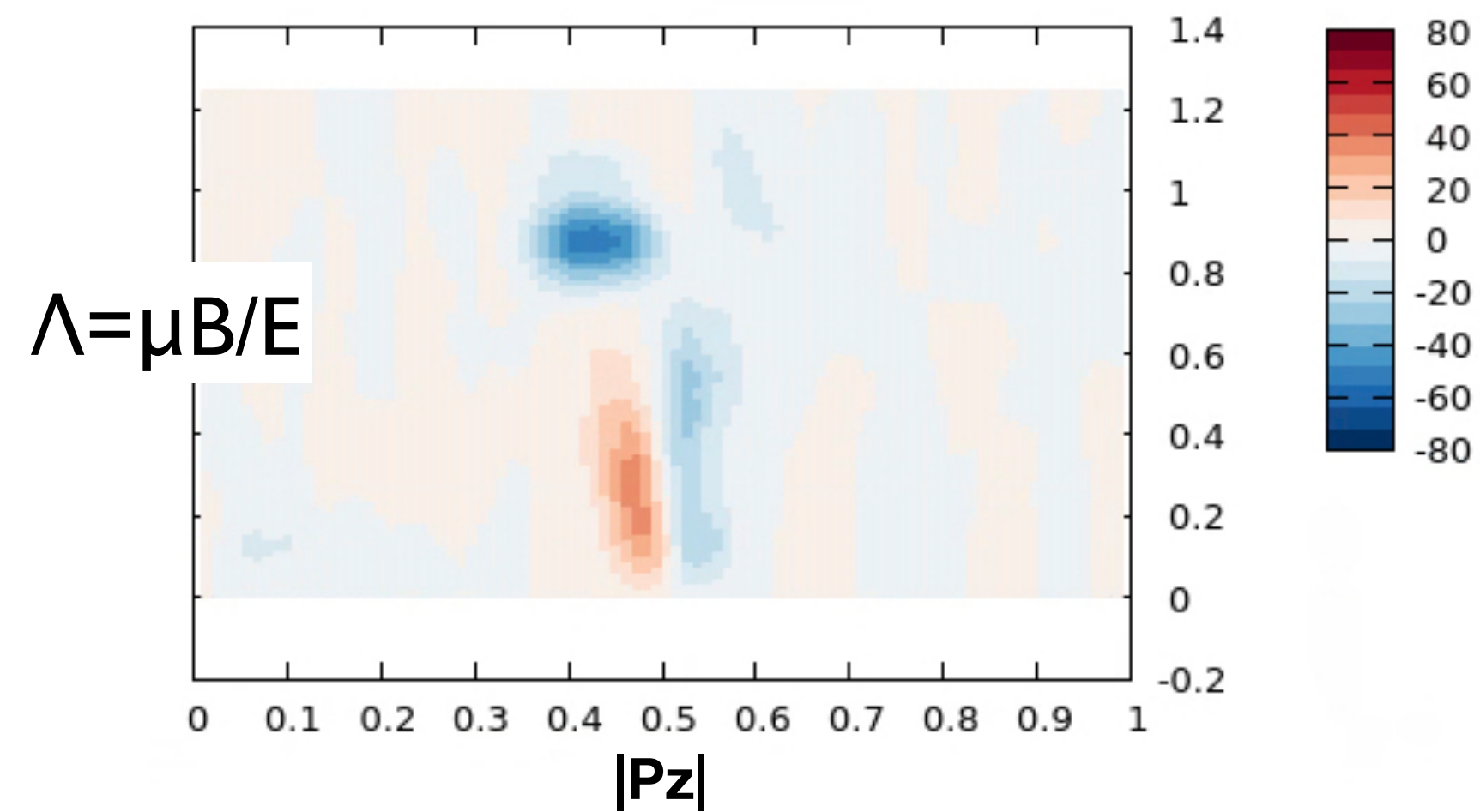


similar for $\langle dE/dt \rangle$

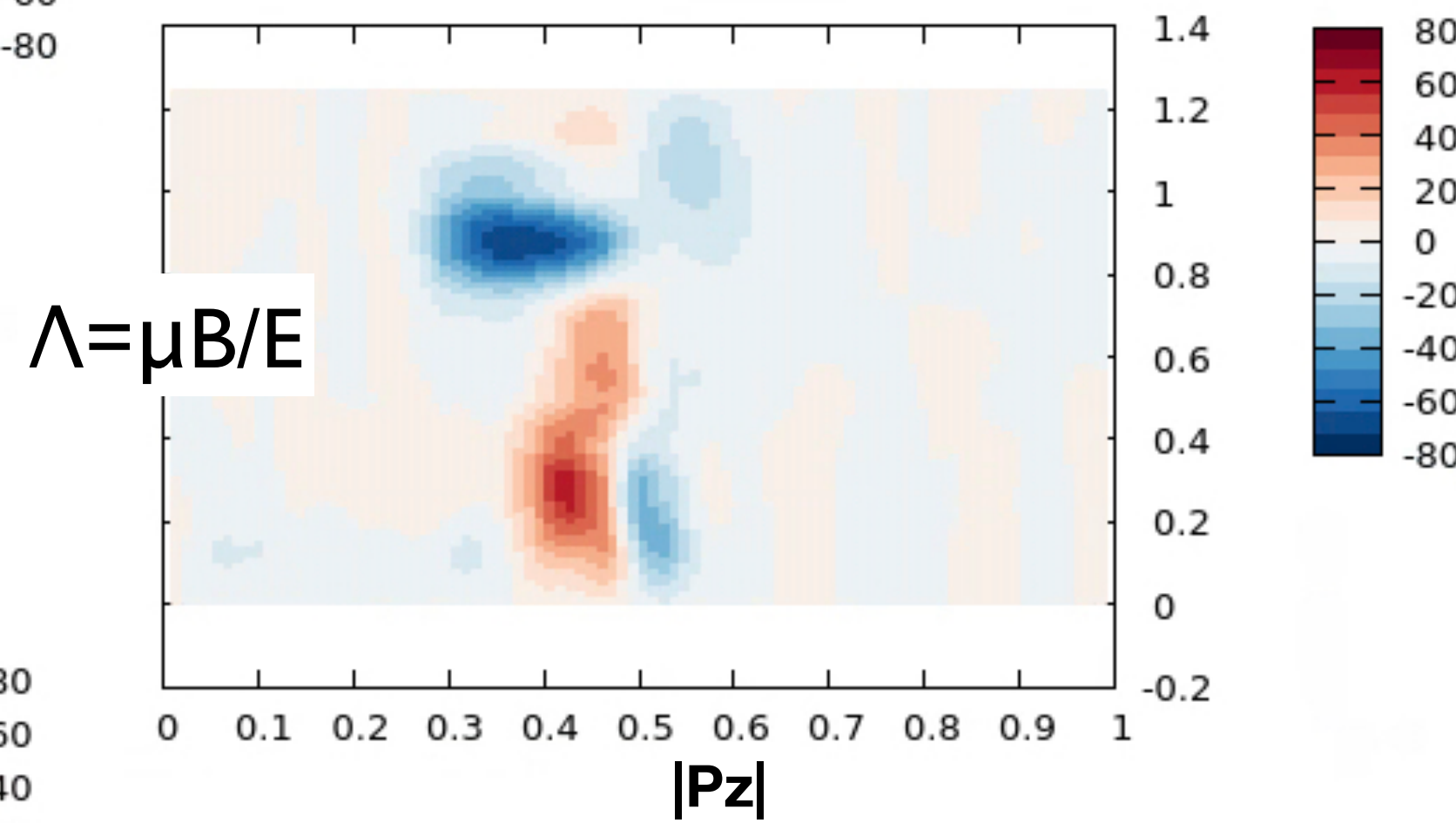
n=16 single



n=17 single

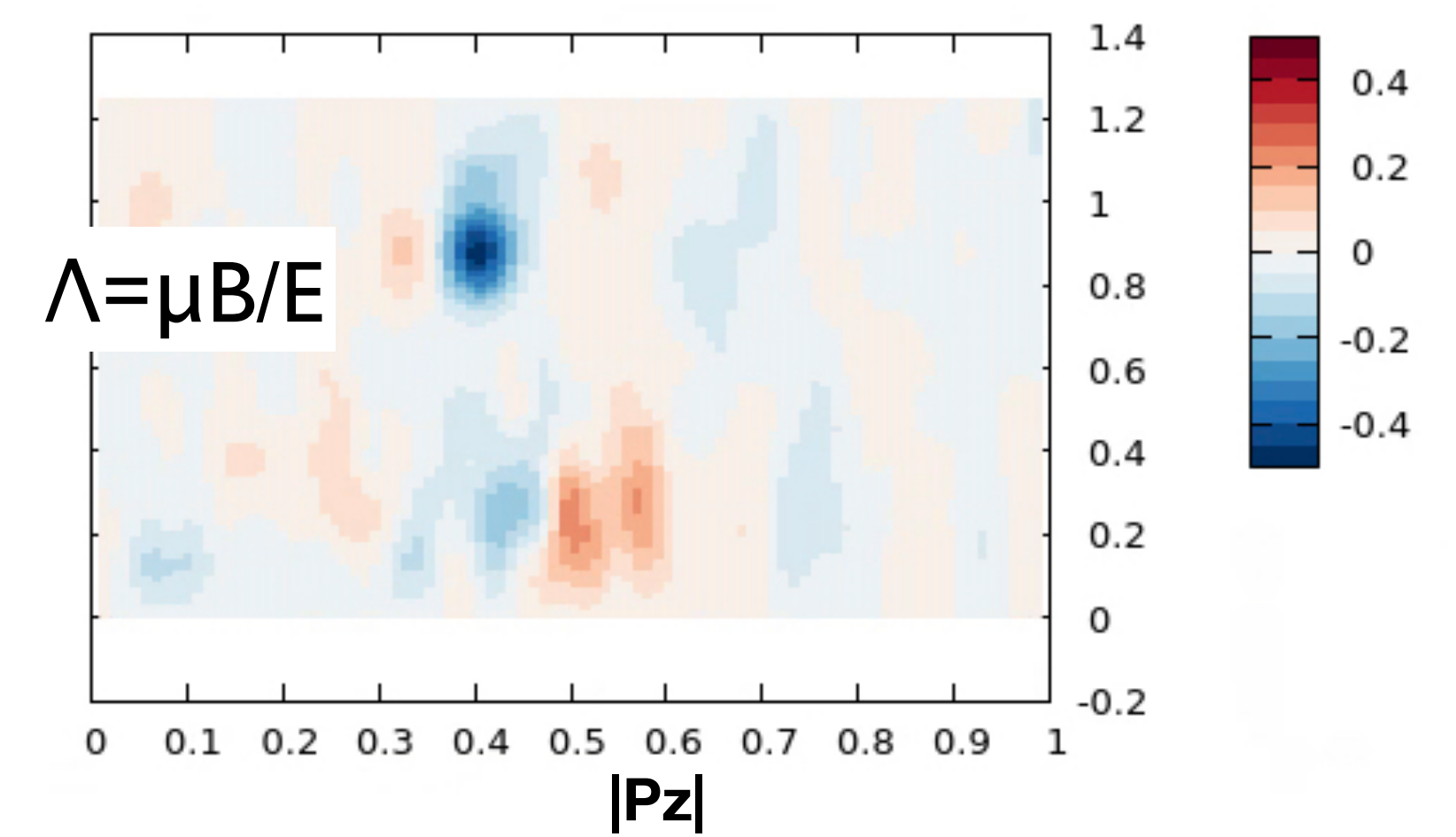


n=16+17 both

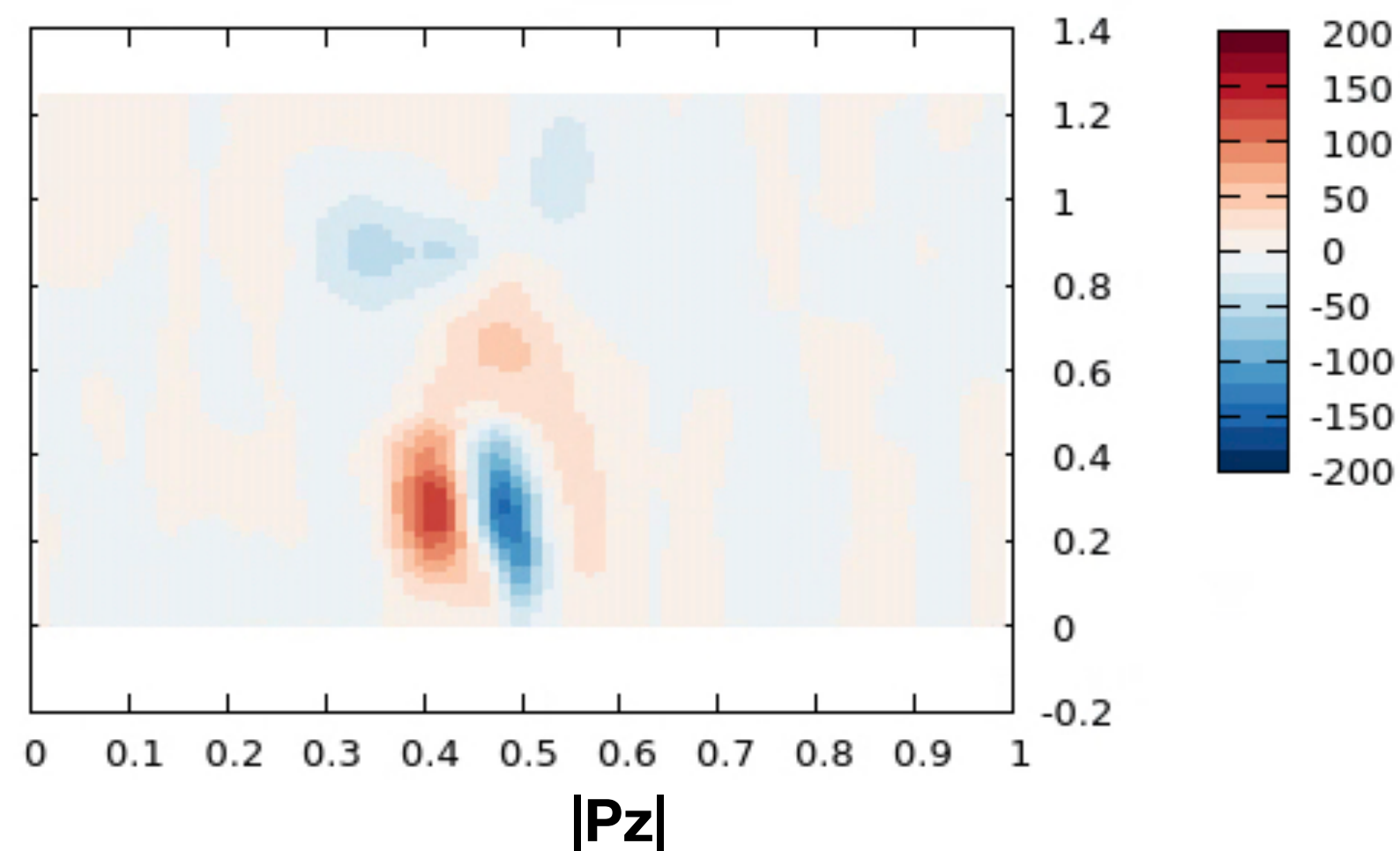


relative difference

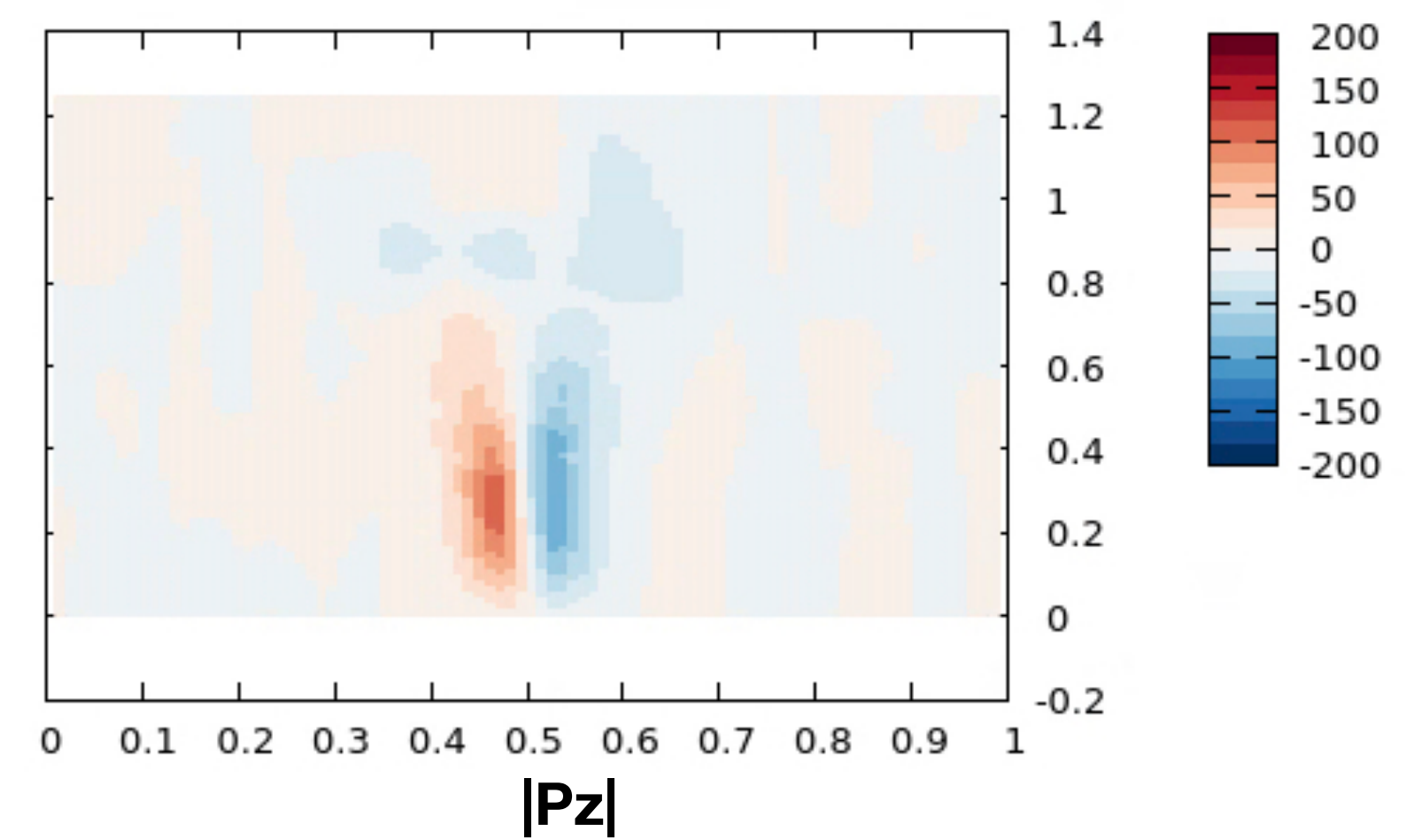
$$\frac{(P_{16+17}) - P(16+17)}{P(16+17)_{\max}}$$



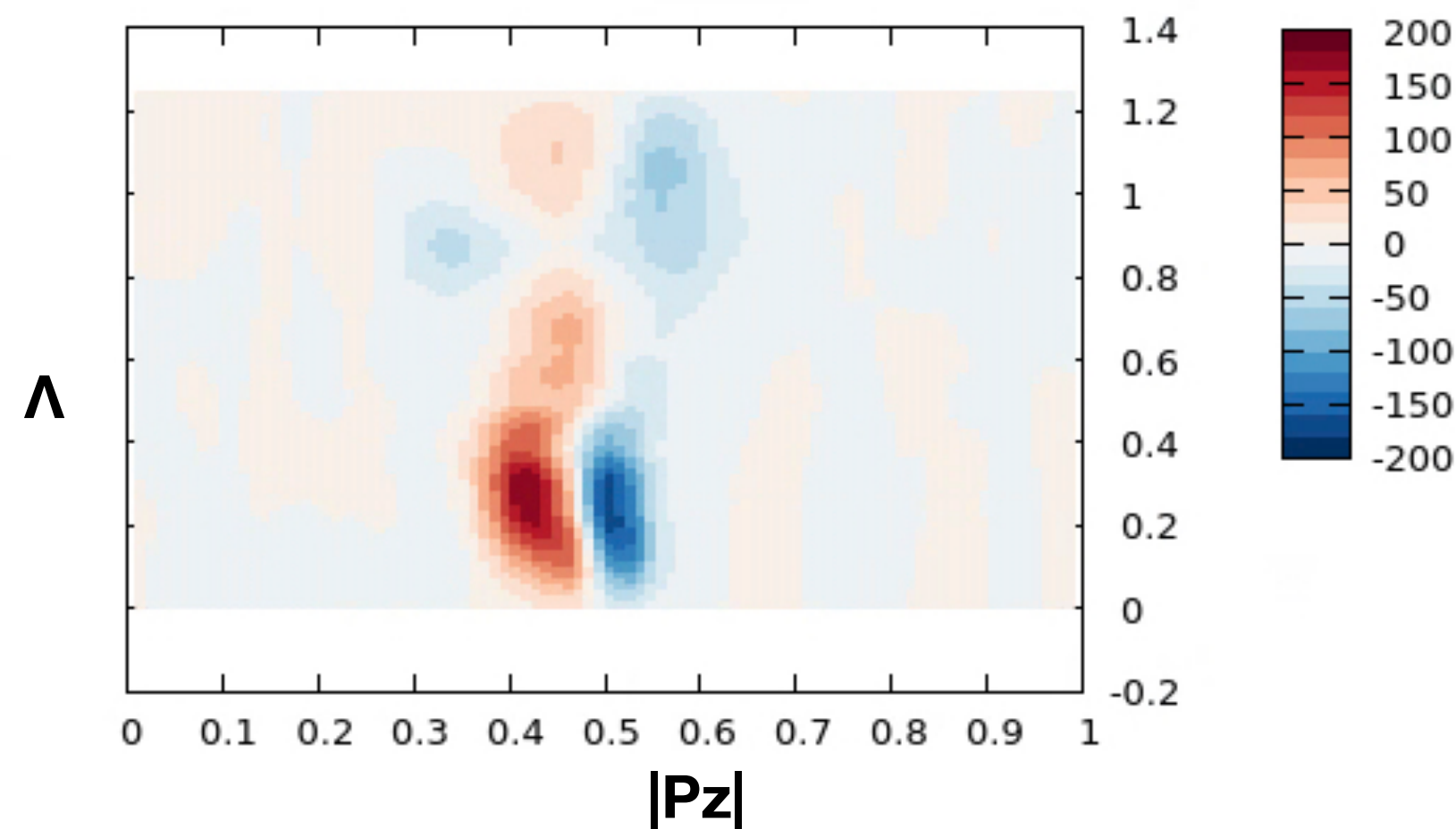
n=16 single



n=17 single

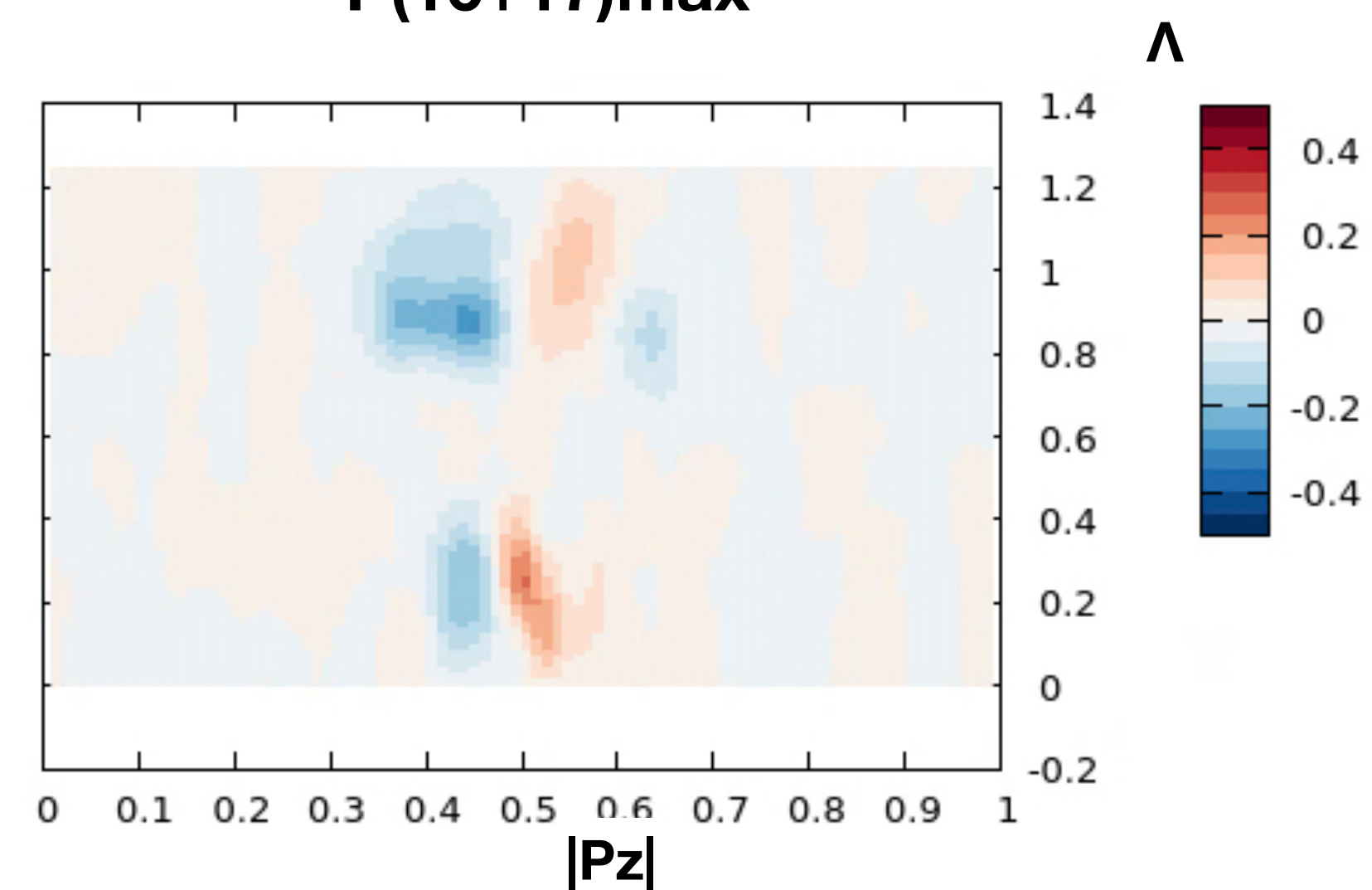


n=16+17 both

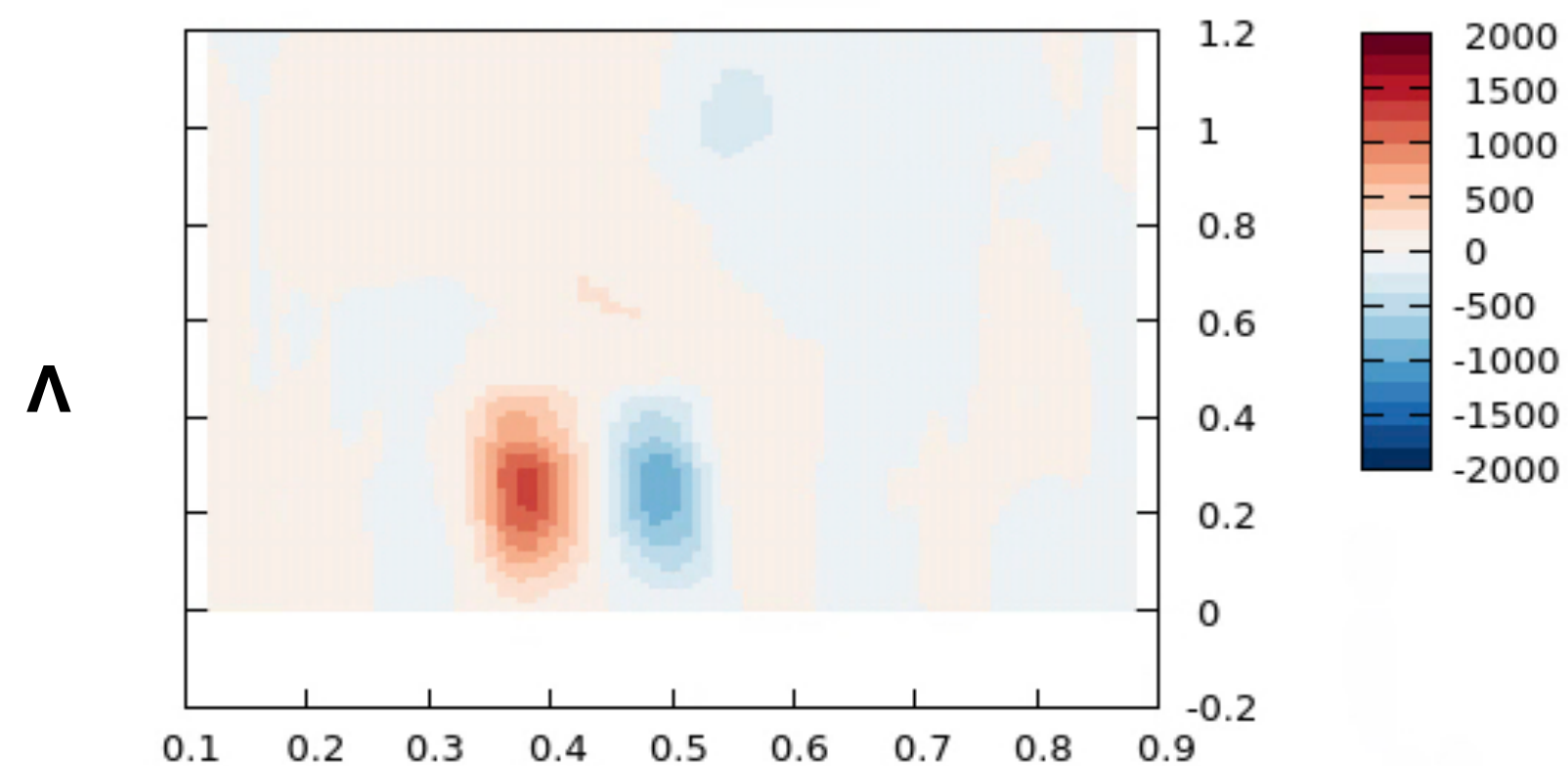


relative difference

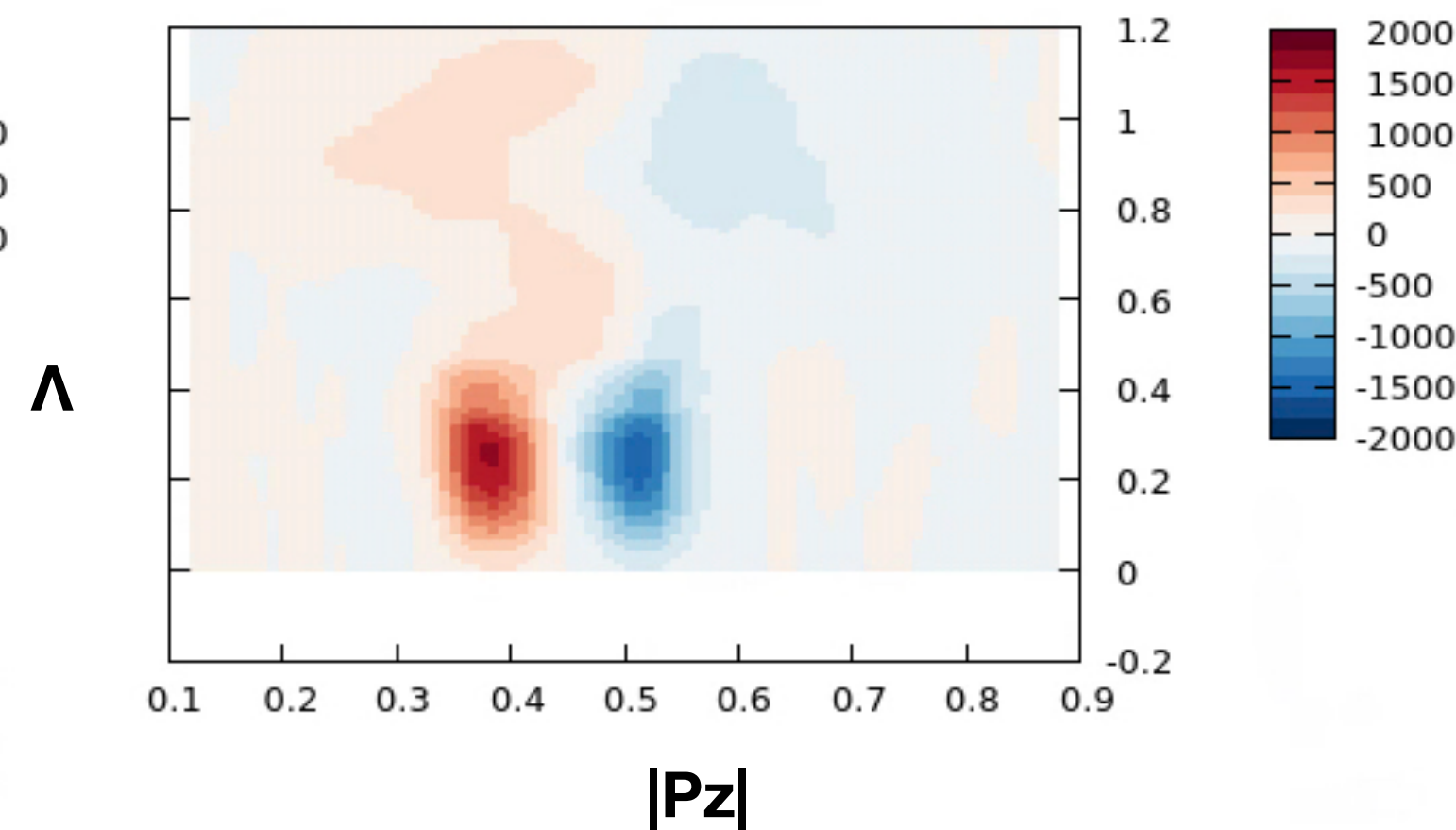
$$\frac{P_{16+17} - P_{(16+17)}}{P_{(16+17)\max}}$$



n=16 single

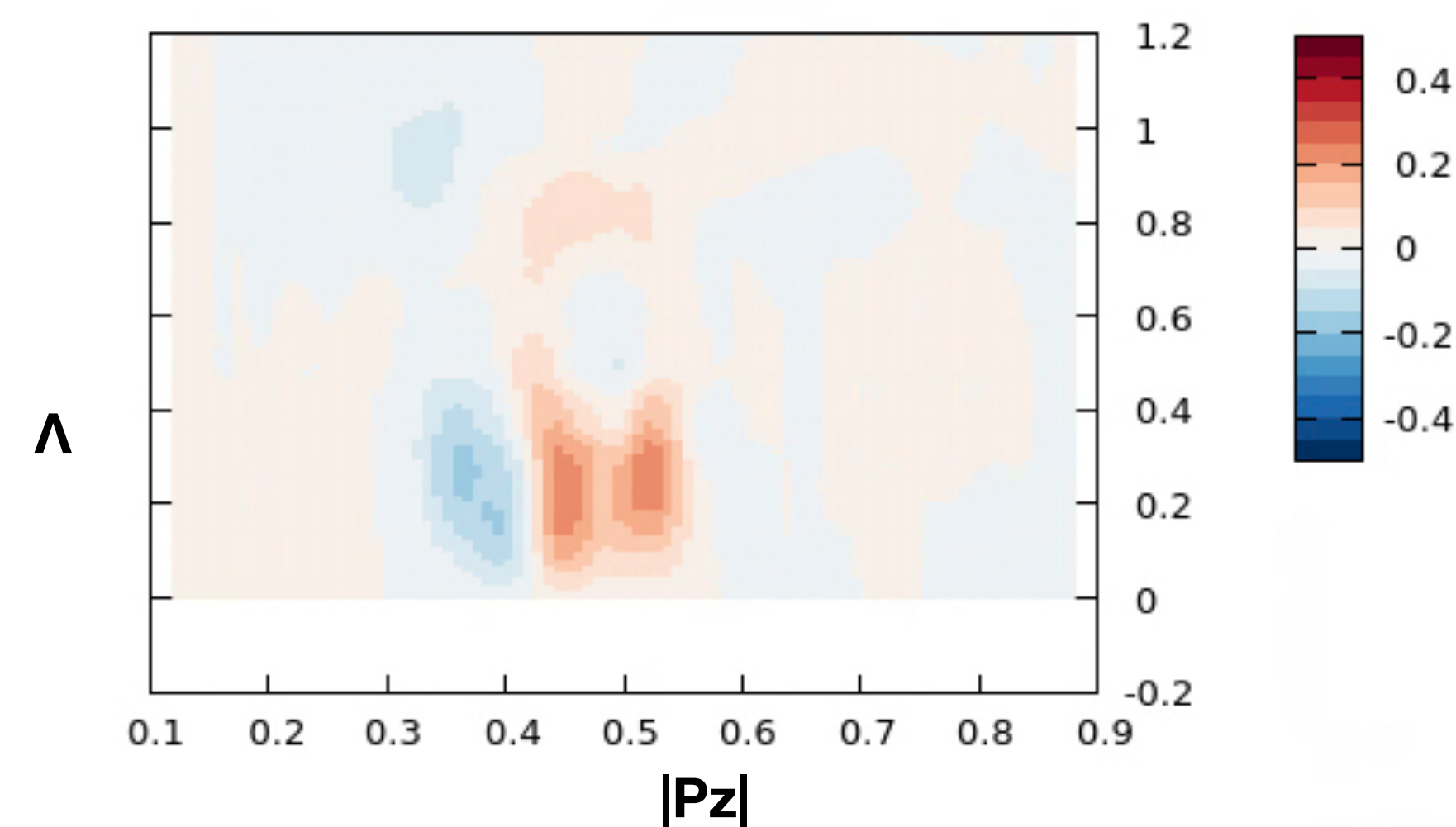


n=16+17 both

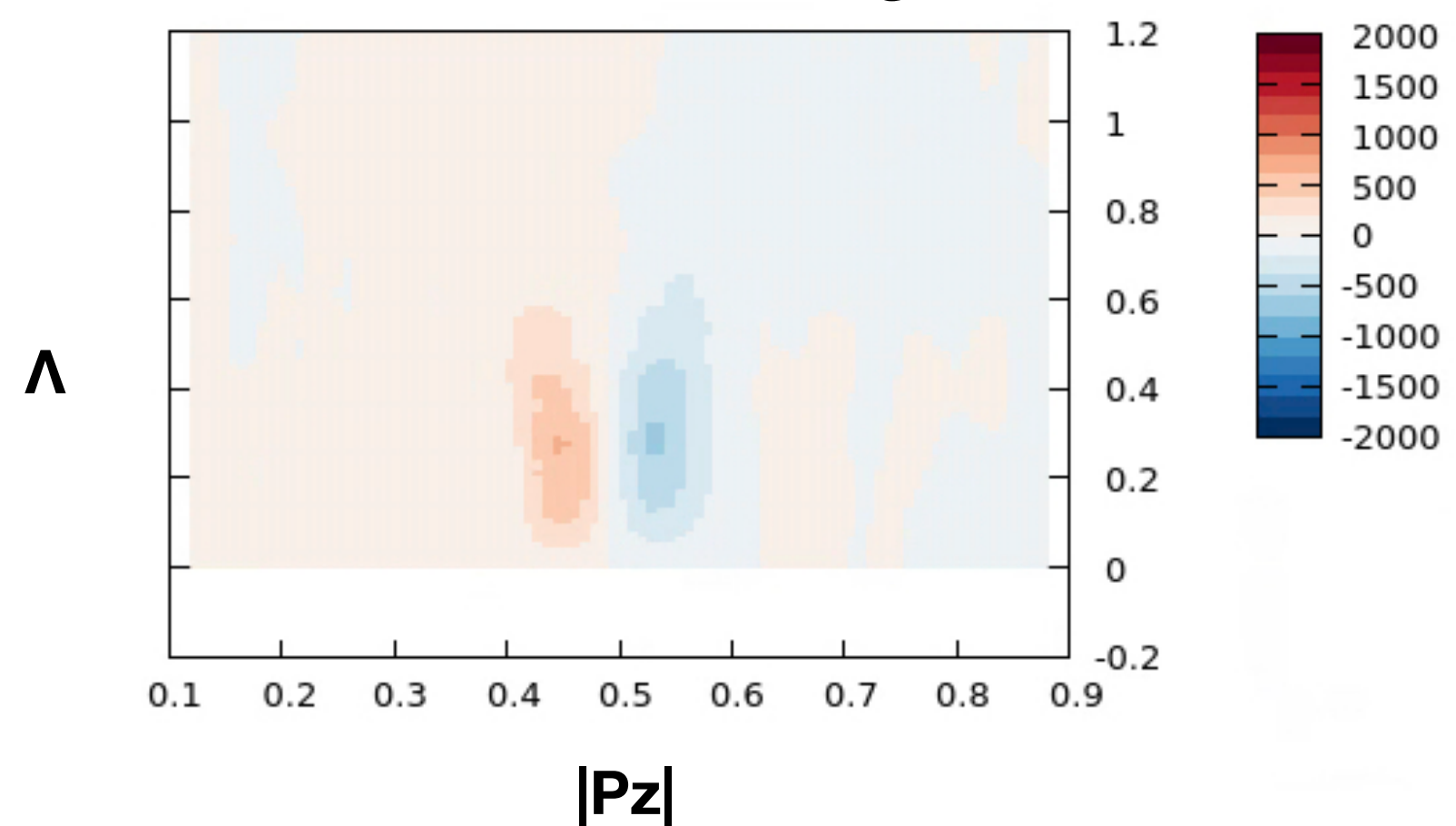


relative difference

$$\frac{P_{16+17} - P(16+17)}{P(16+17)_{\max}}$$



|Pz| n=17 single



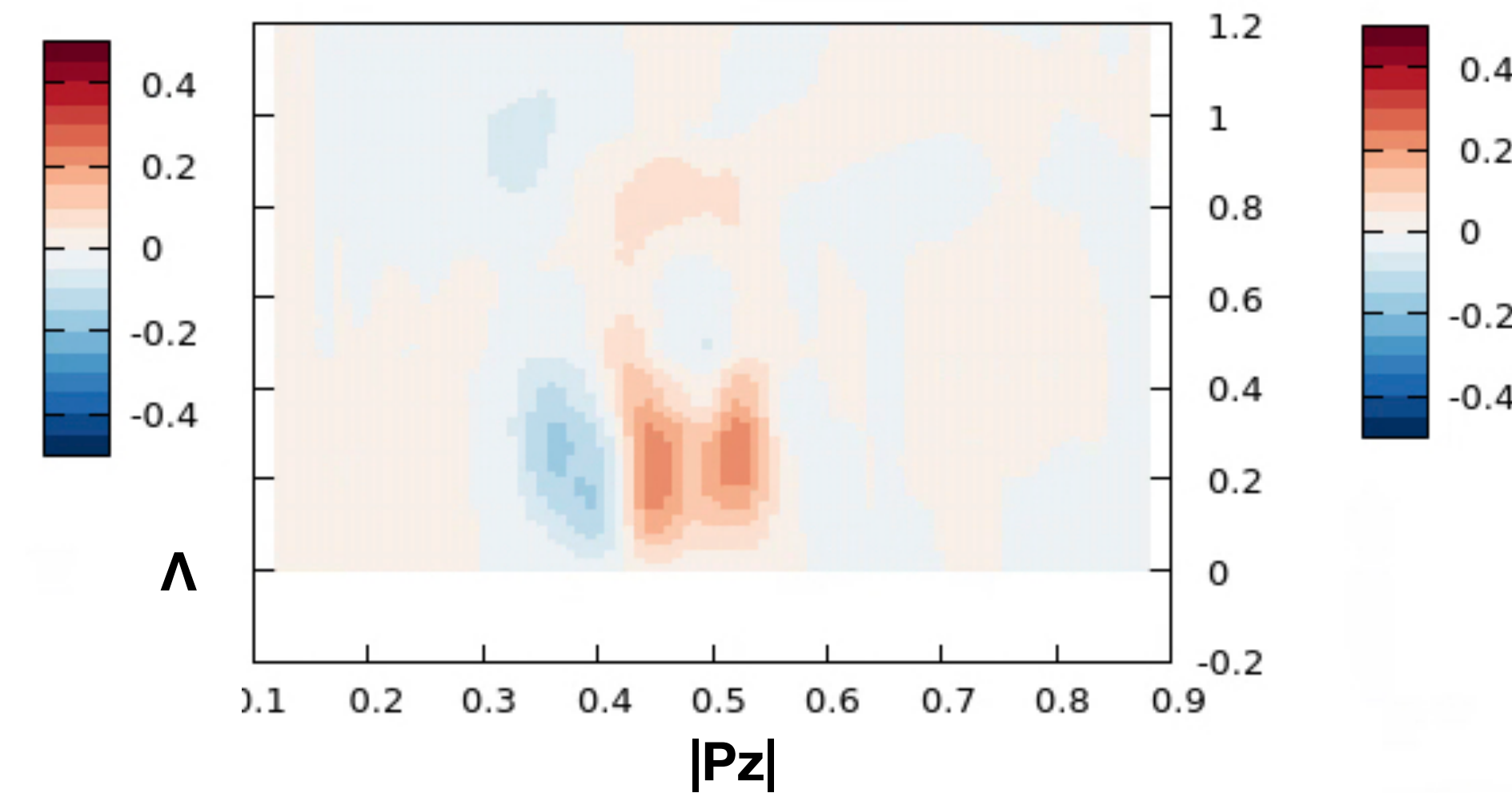
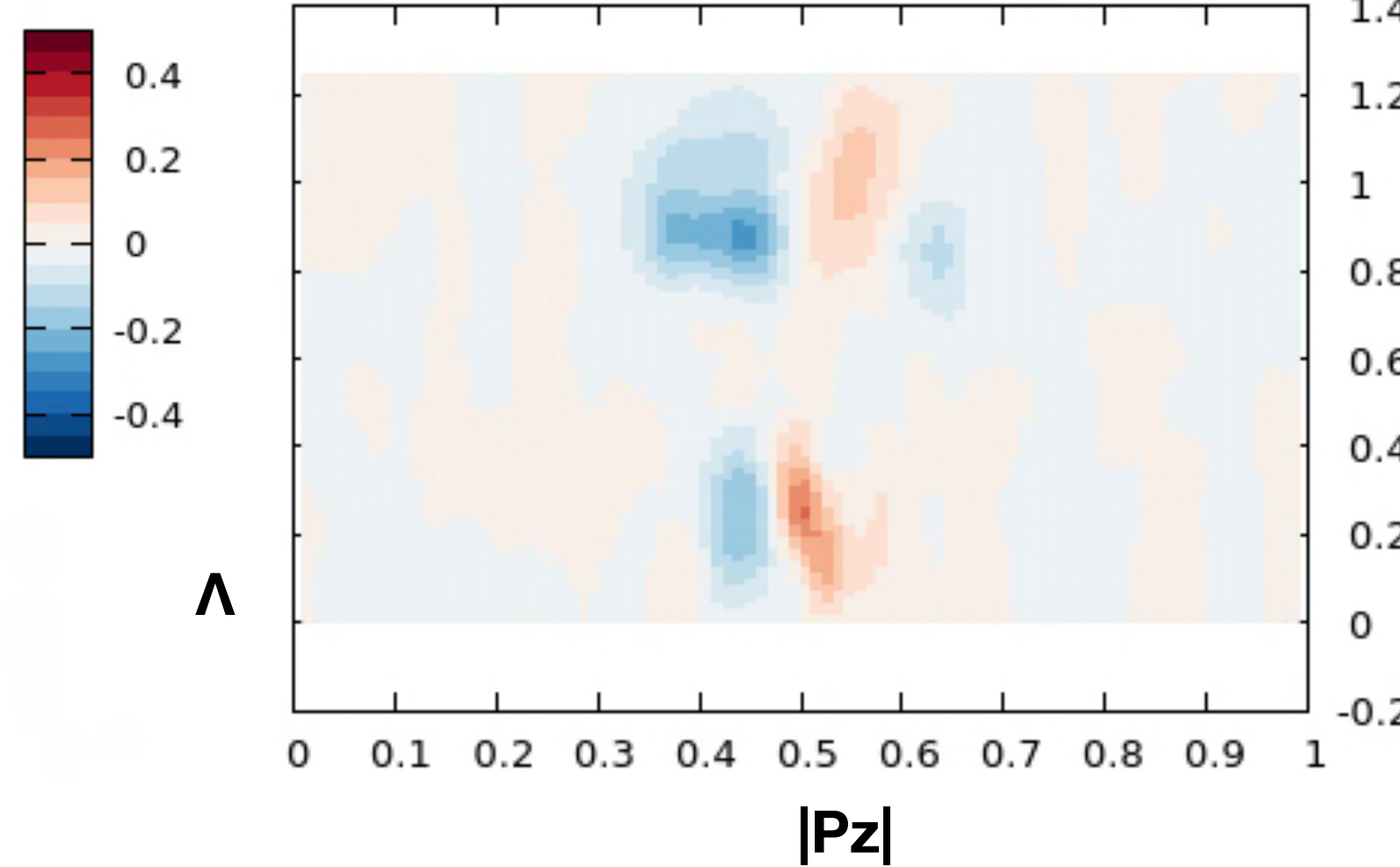
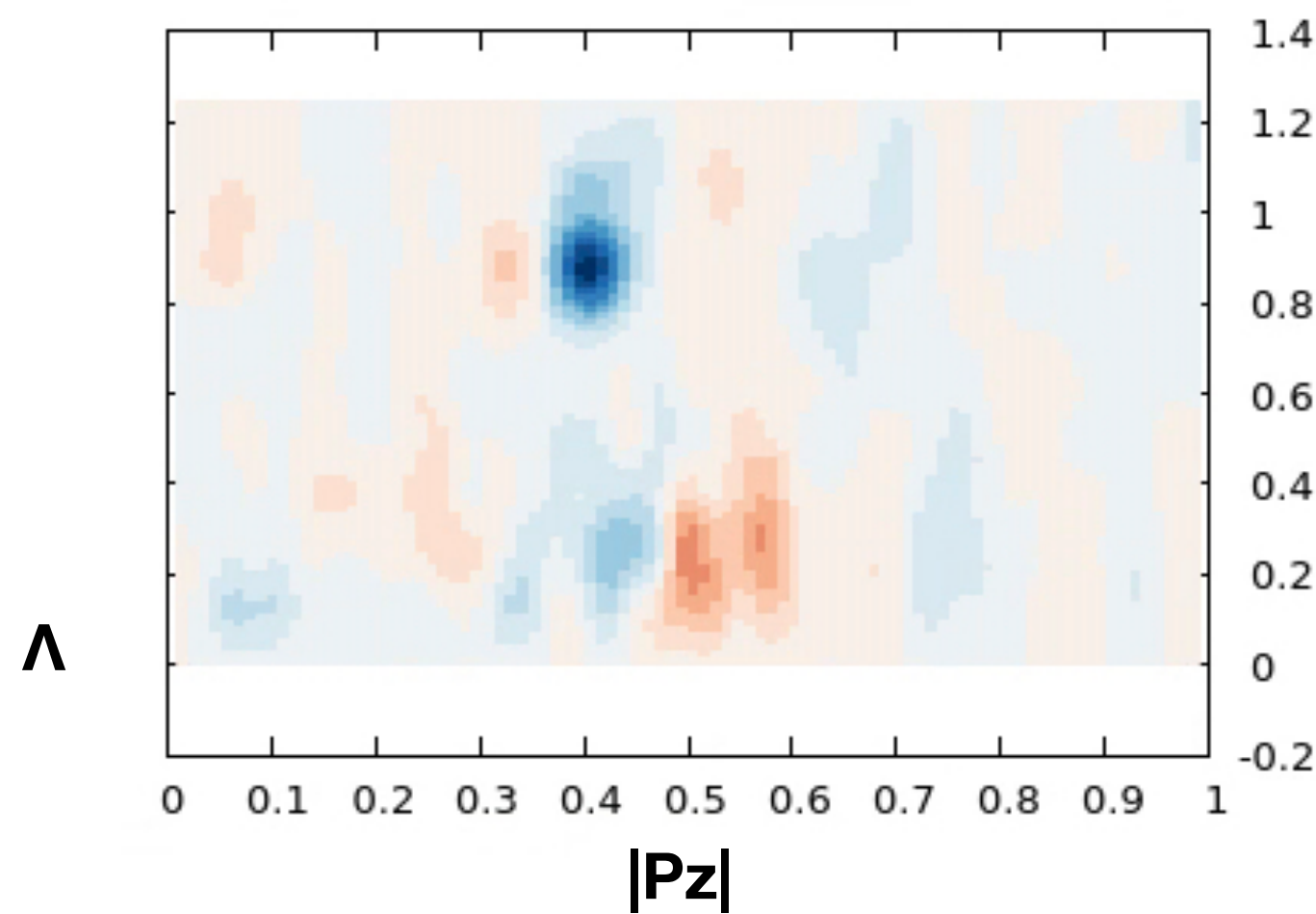
start to investigate multi-mode cases: amplitude scan

relative difference $\frac{(P_{16+P17})-P(16+17)}{P(16+17)_{max}}$

$dB/B=0.5 * 10^{-3}$

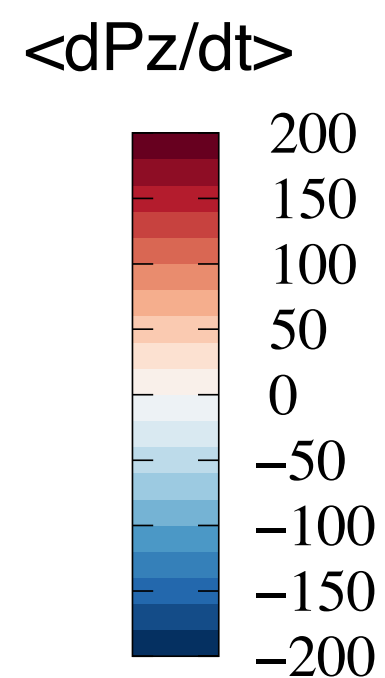
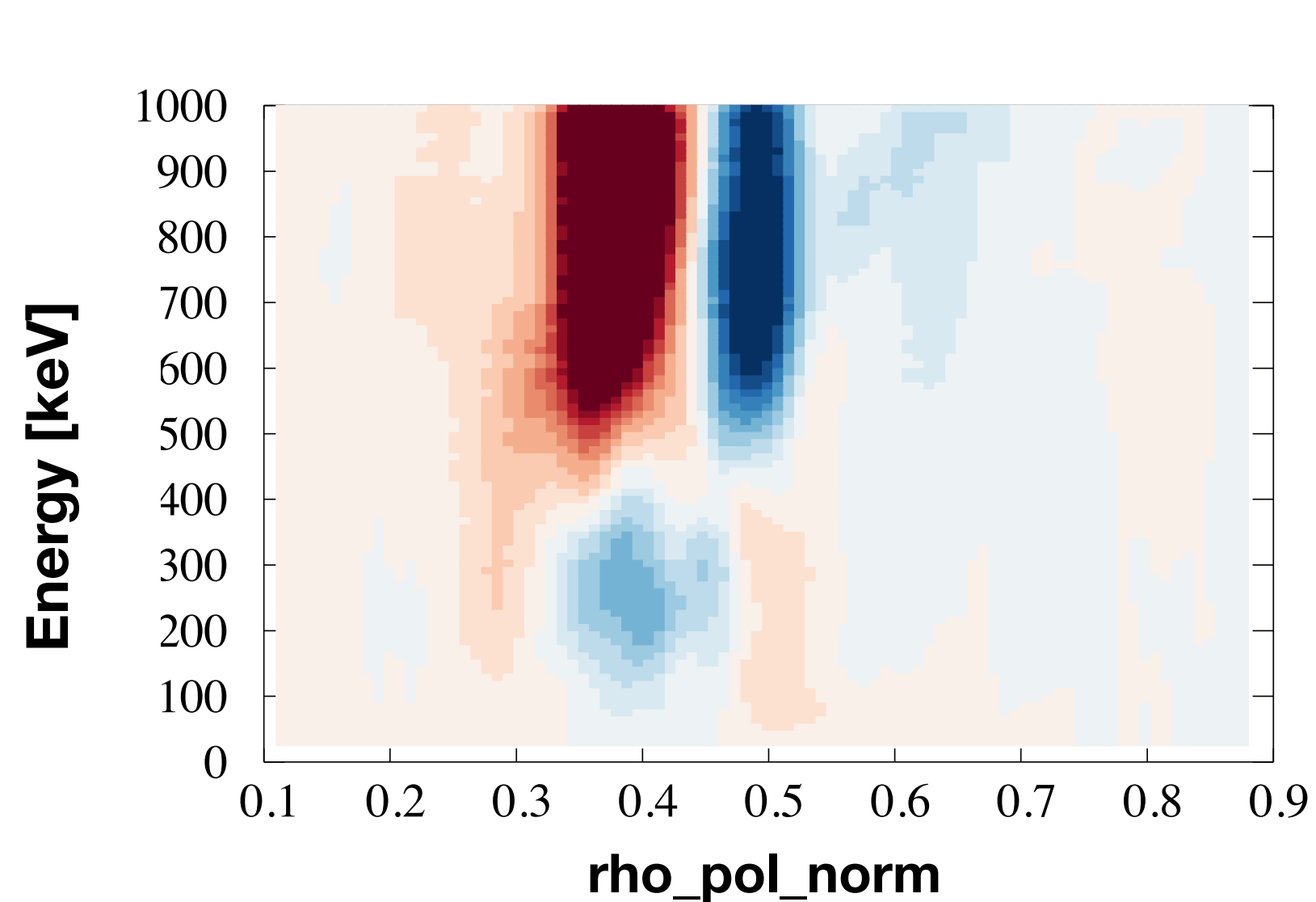
$dB/B=1 * 10^{-3}$

$dB/B=5 * 10^{-3}$

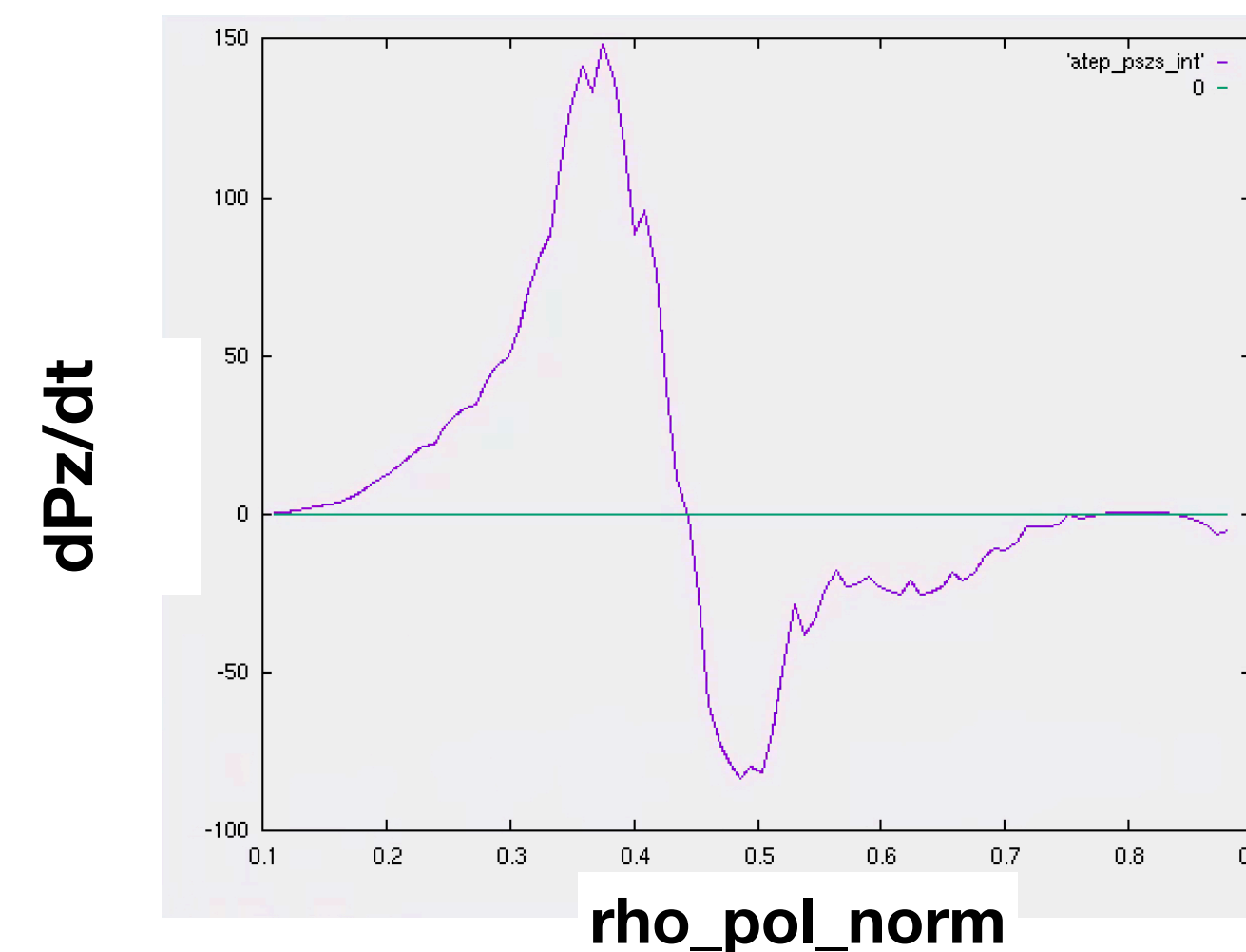


- multi-mode systems need careful treatment when going from isolated mode case to resonance-overlap (diffusive) regime:
- depending on amplitude, trapped and passing particles show different relative importance for causing resonance overlap (FOW vs resonance width)
- example shows capability of model to check assumptions, understand underlying physics and to trigger next level of model hierarchy, if necessary

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



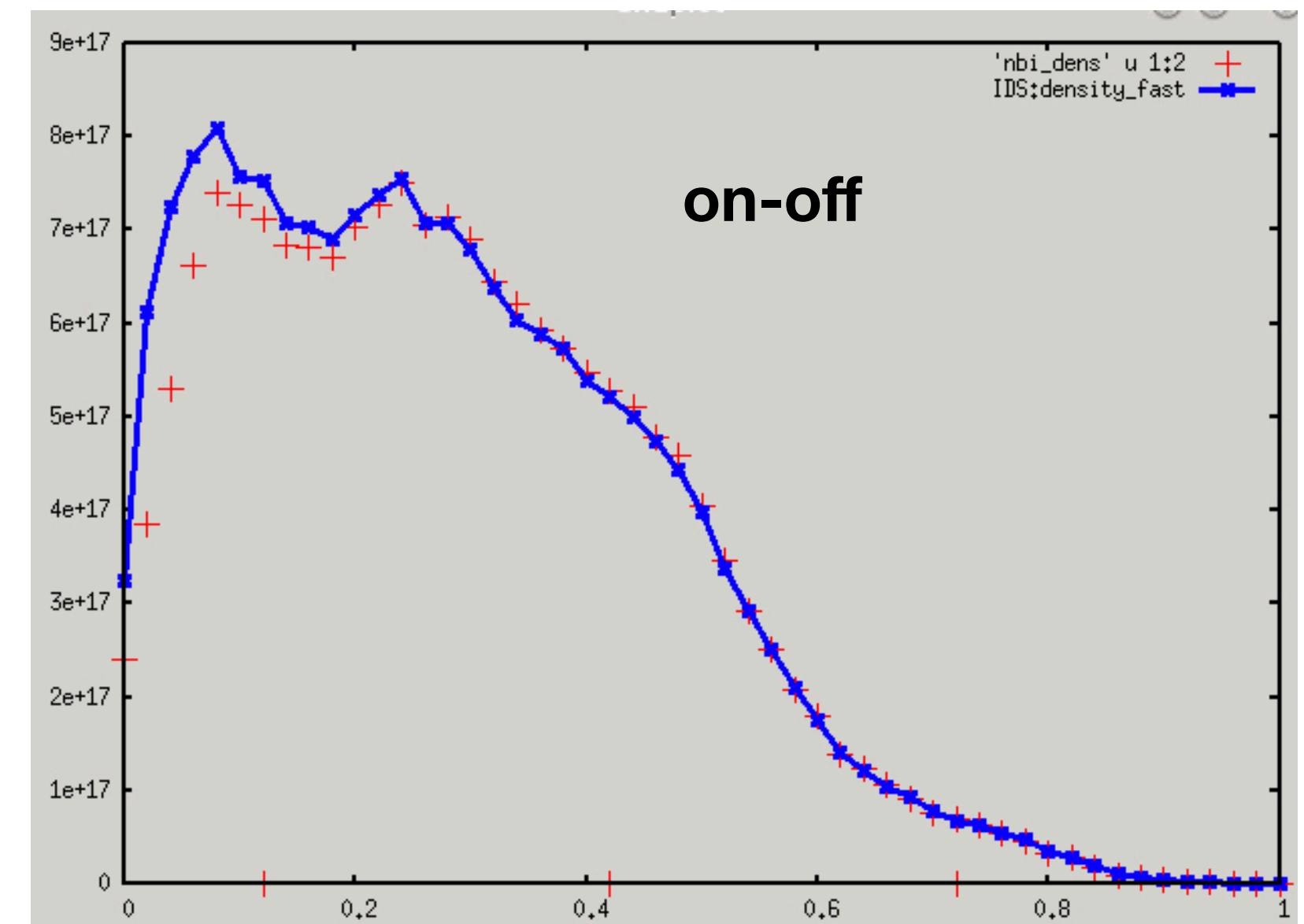
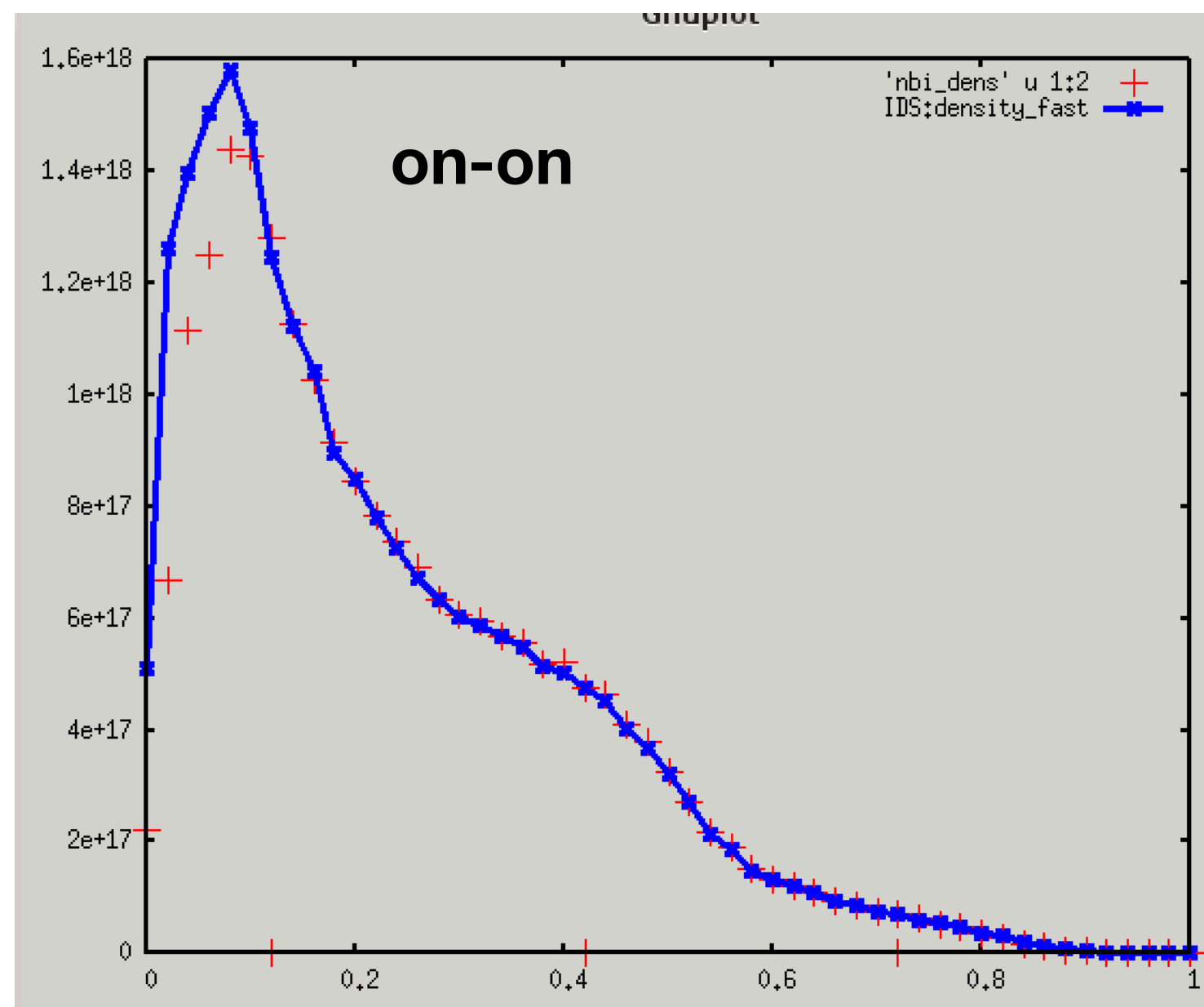
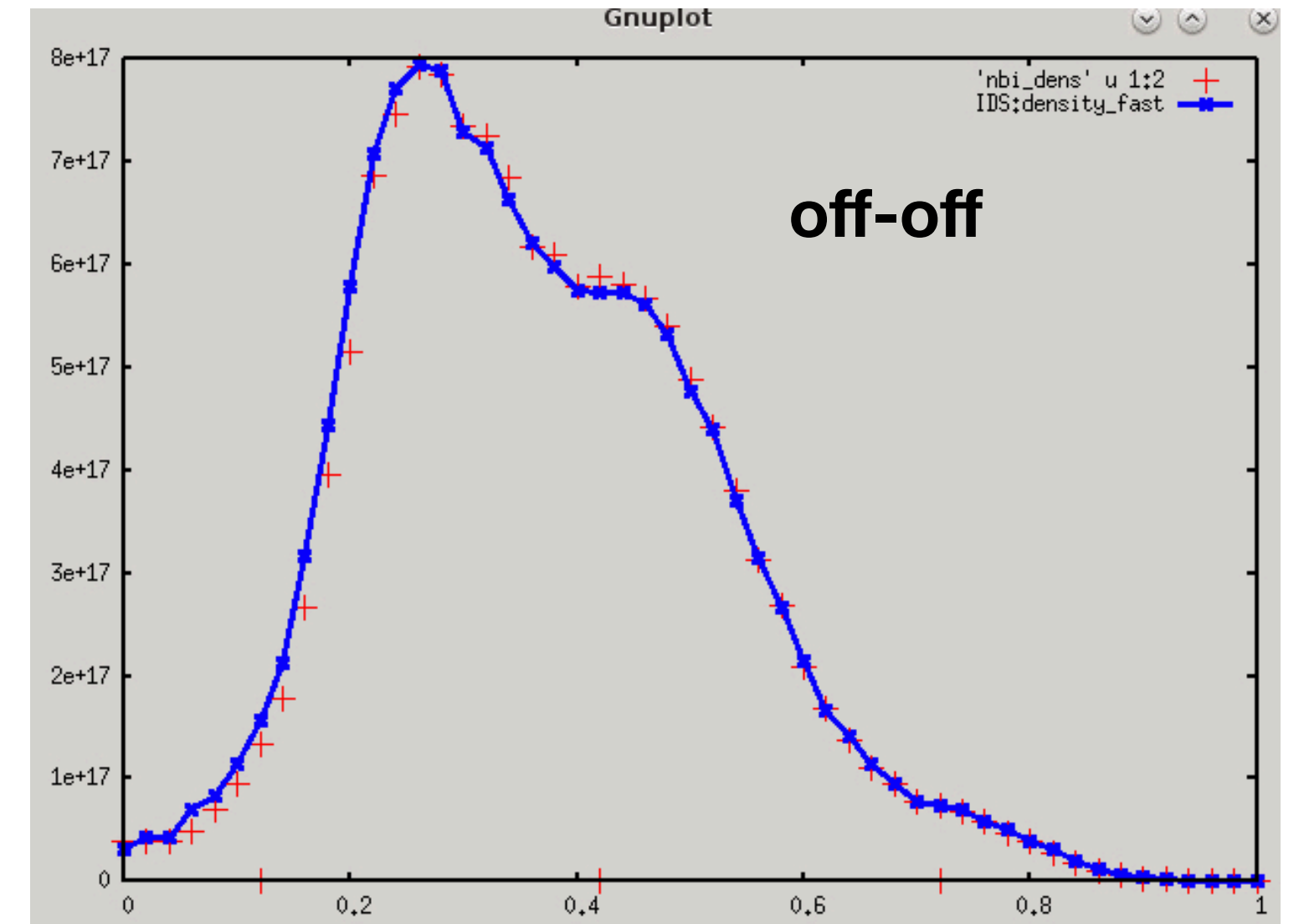
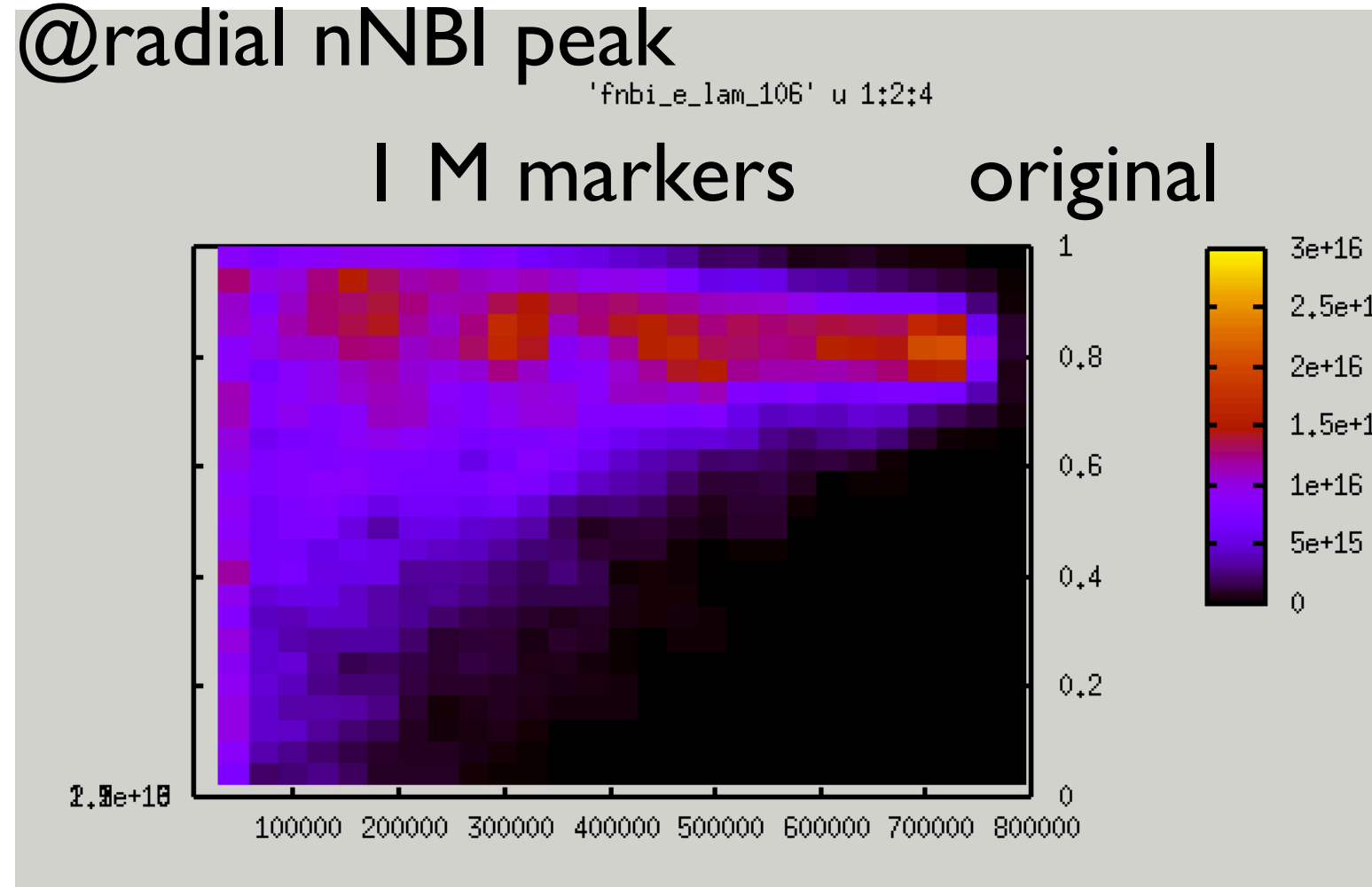
E integration
→



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

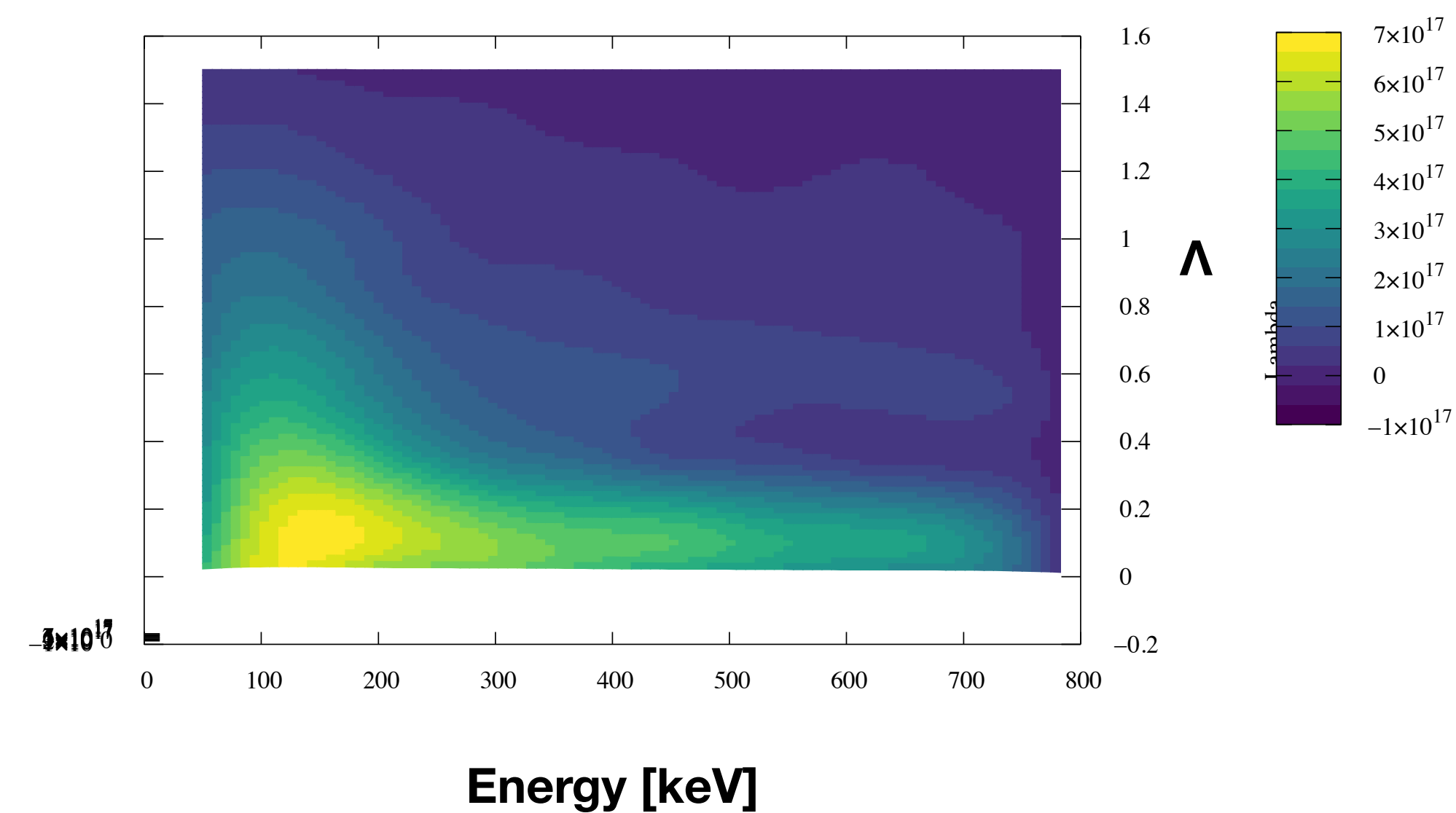
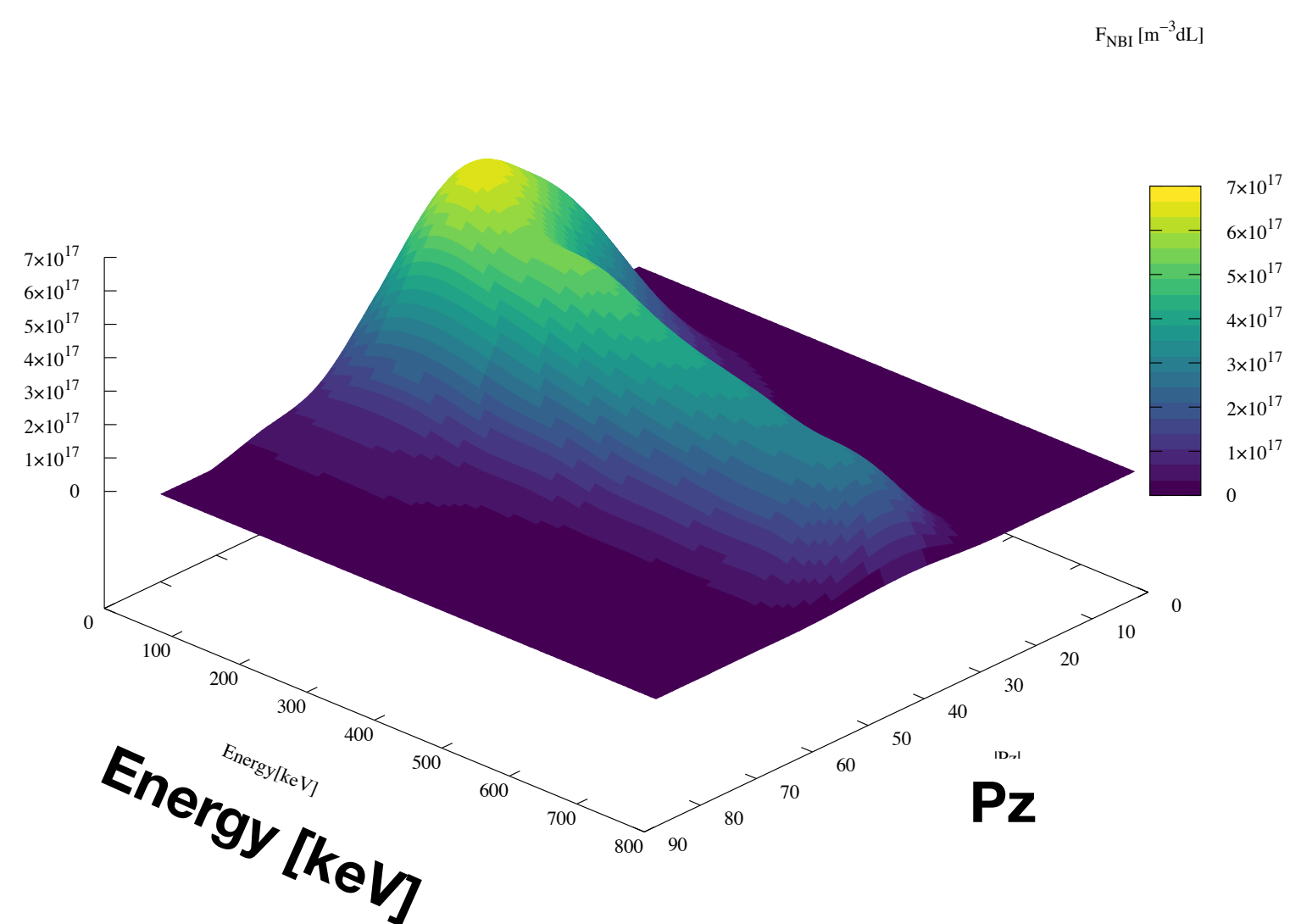
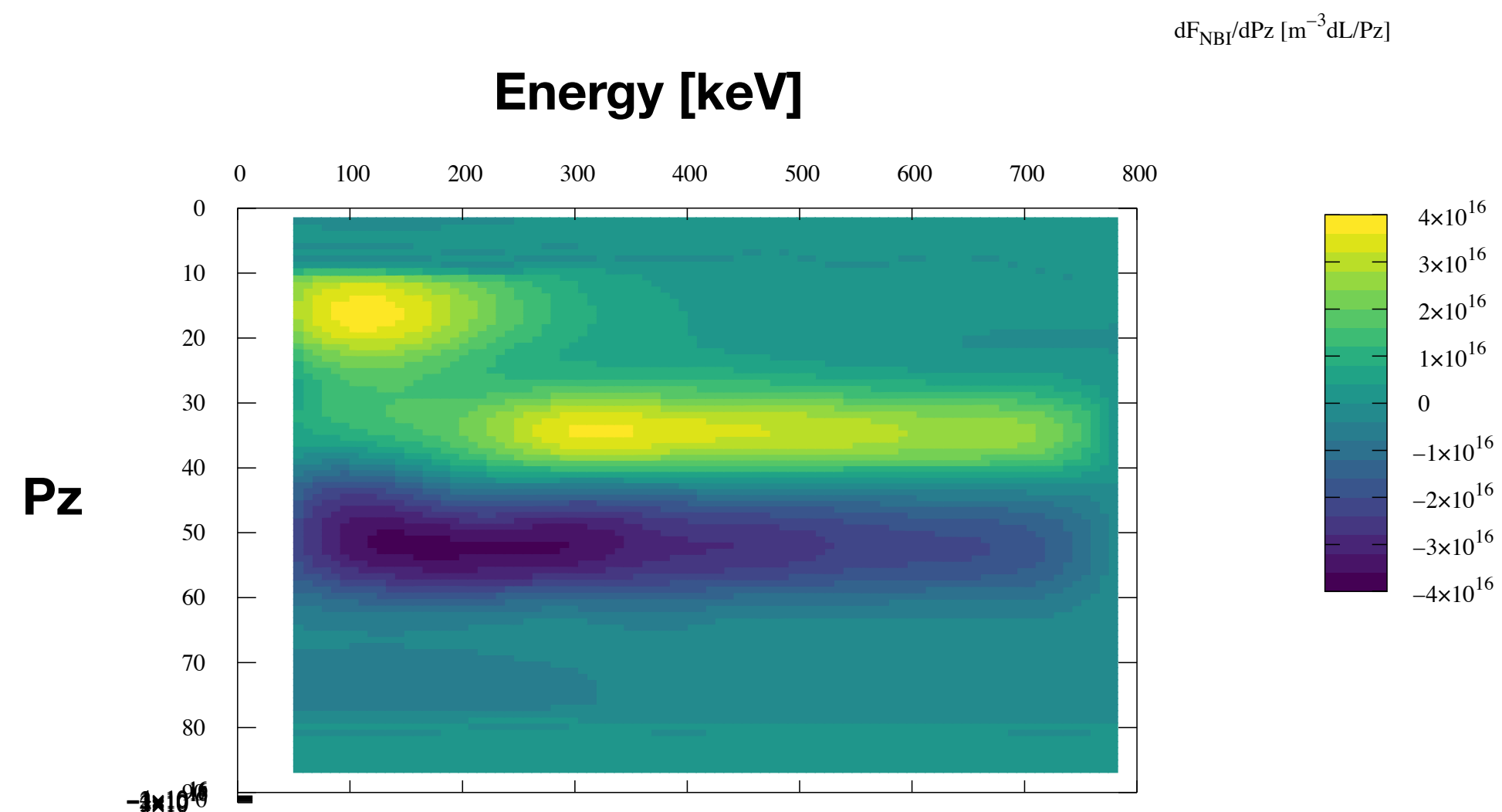
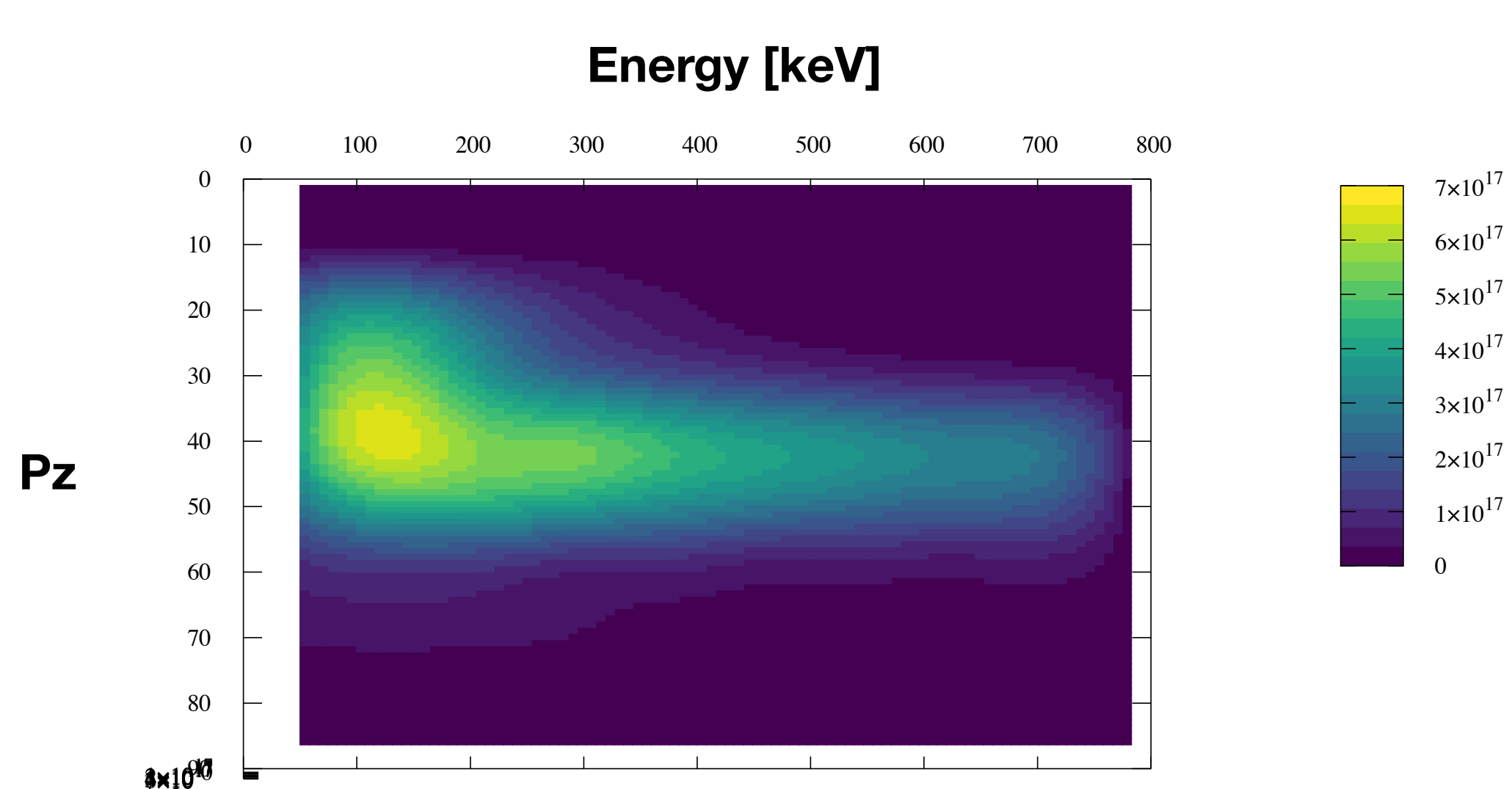


progress on implementation of transport model: ATEP code



bin/smooth/map to same COM grid as PSZS

binning I 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):

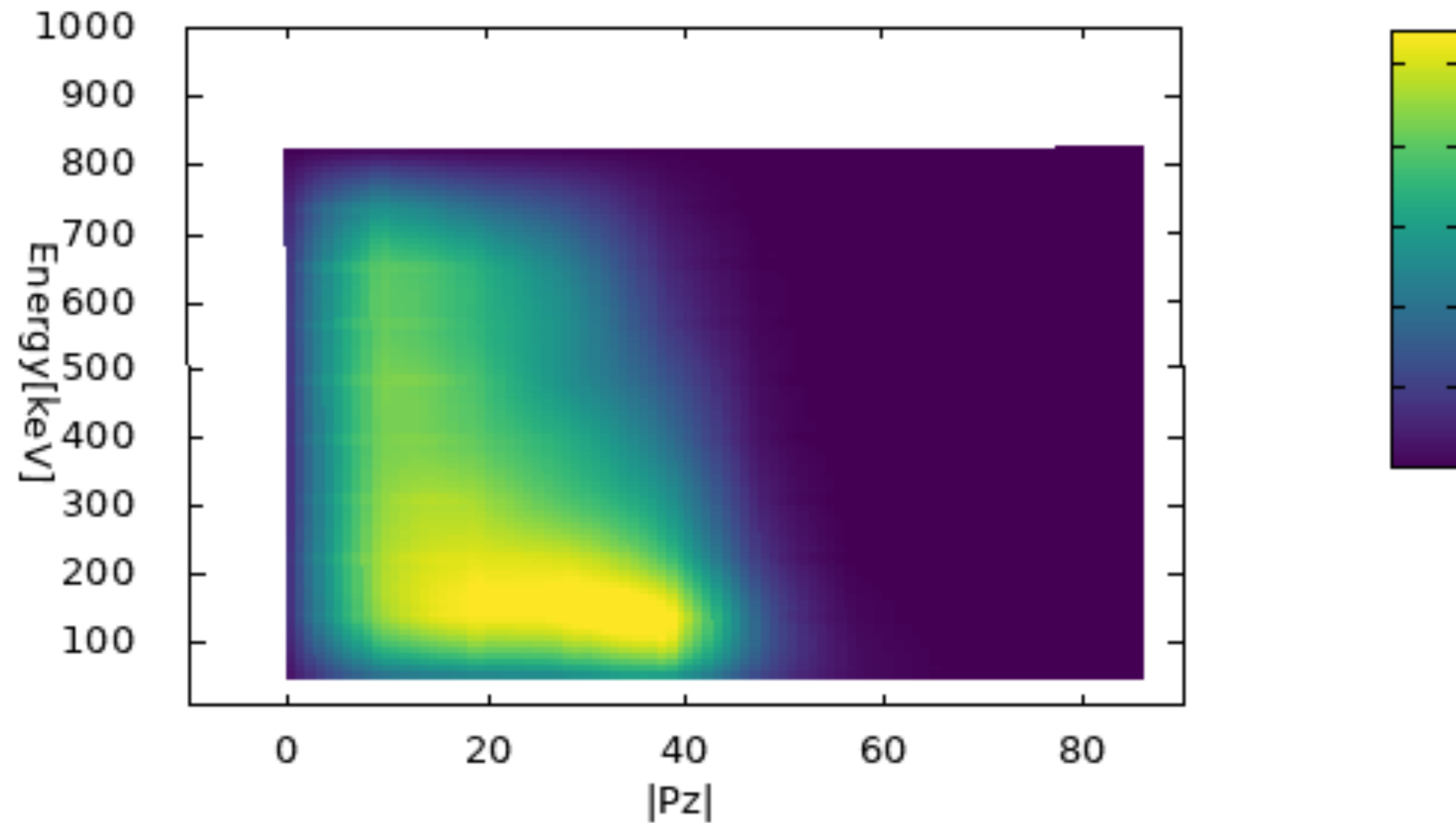
$$\frac{\partial F_{EP}}{\partial t} = \frac{\partial P_z}{\partial t} \frac{\partial F_{EP}}{\partial P_z} + \frac{\partial E}{\partial t} \frac{\partial F_{EP}}{\partial E}$$

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

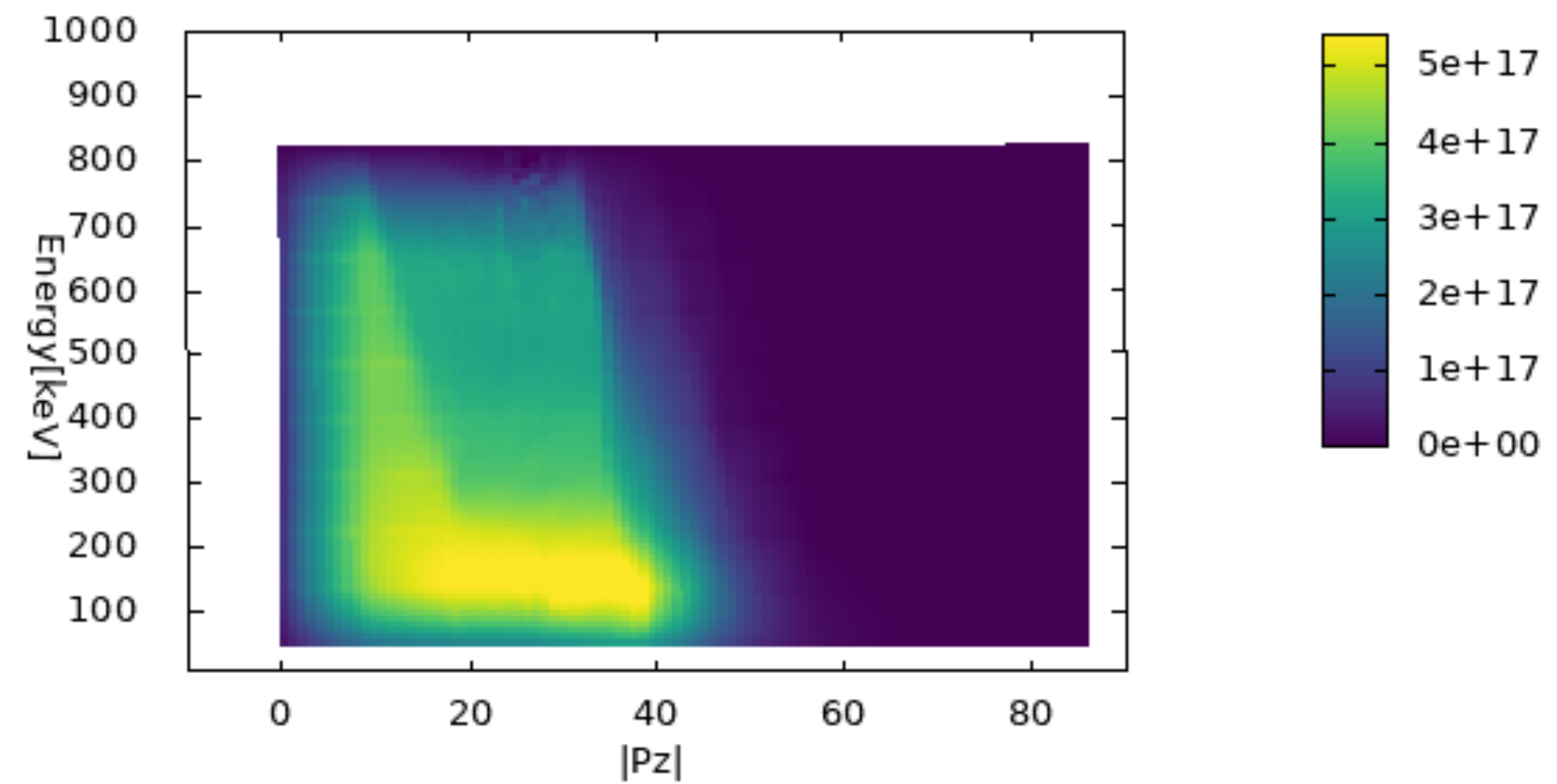
runtime: several seconds

FEP at start:

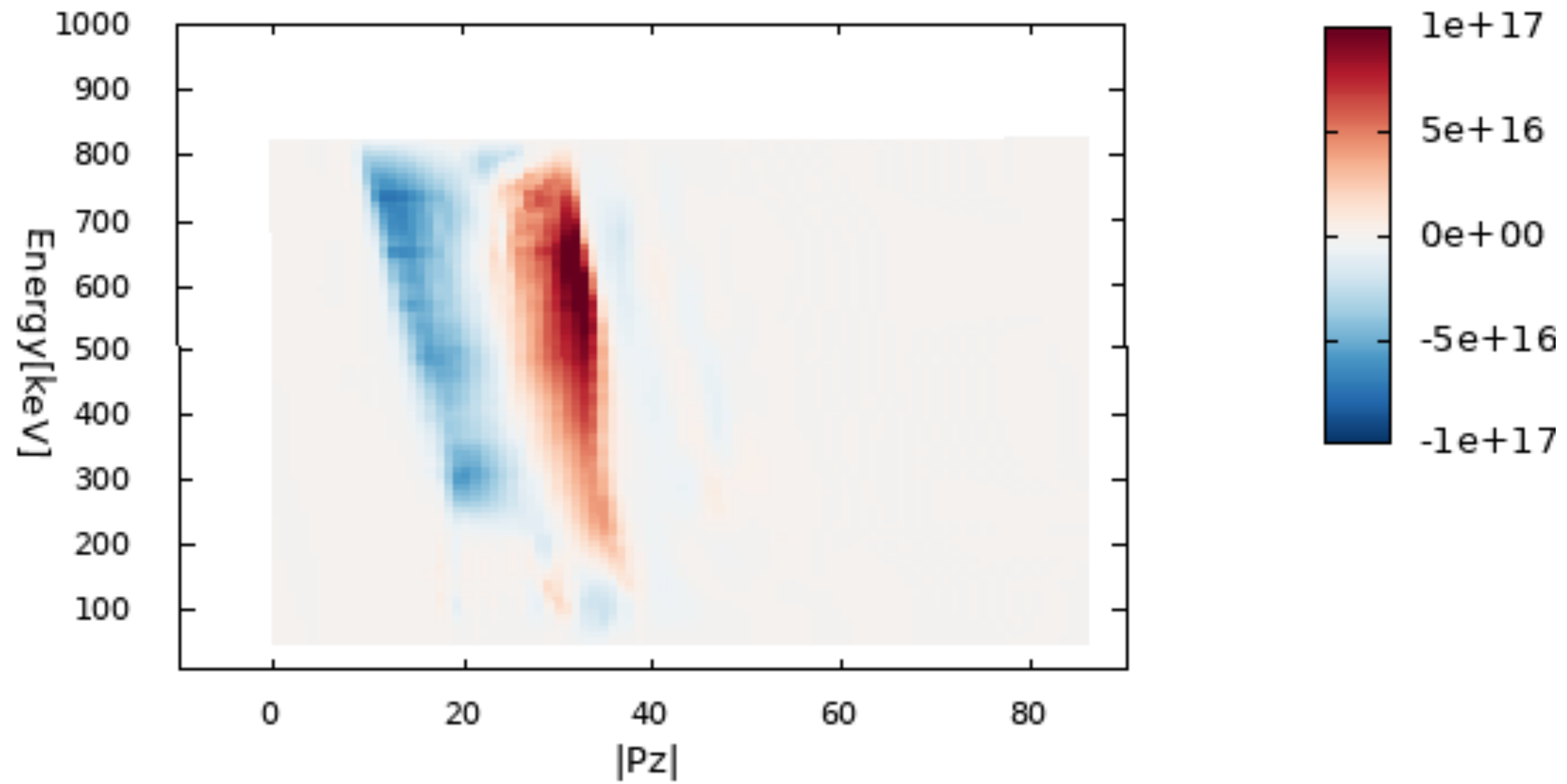
F (Pz,E,t), Time=2 [arb units]



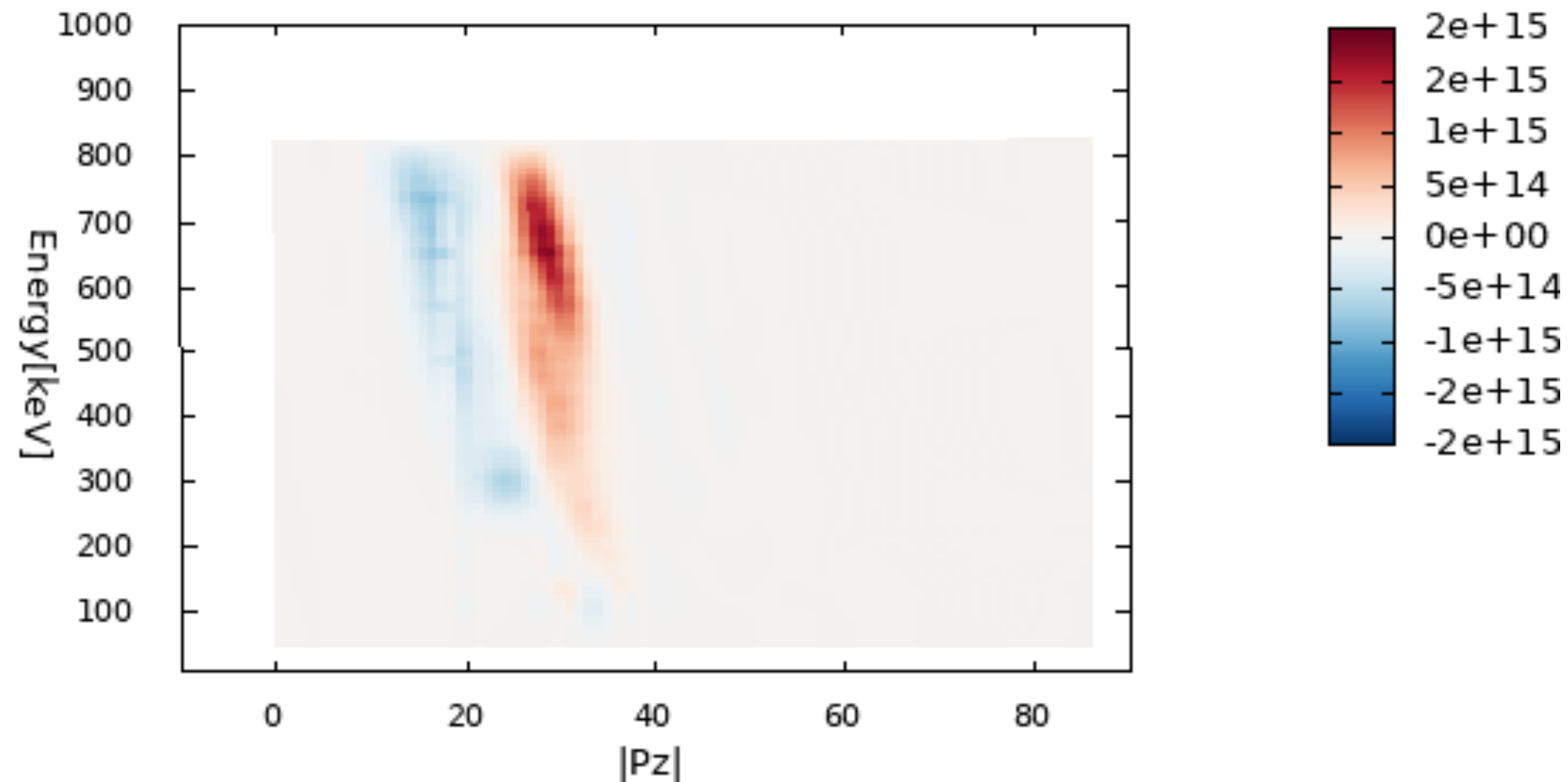
F (Pz,E,t), Time=199 [arb units]



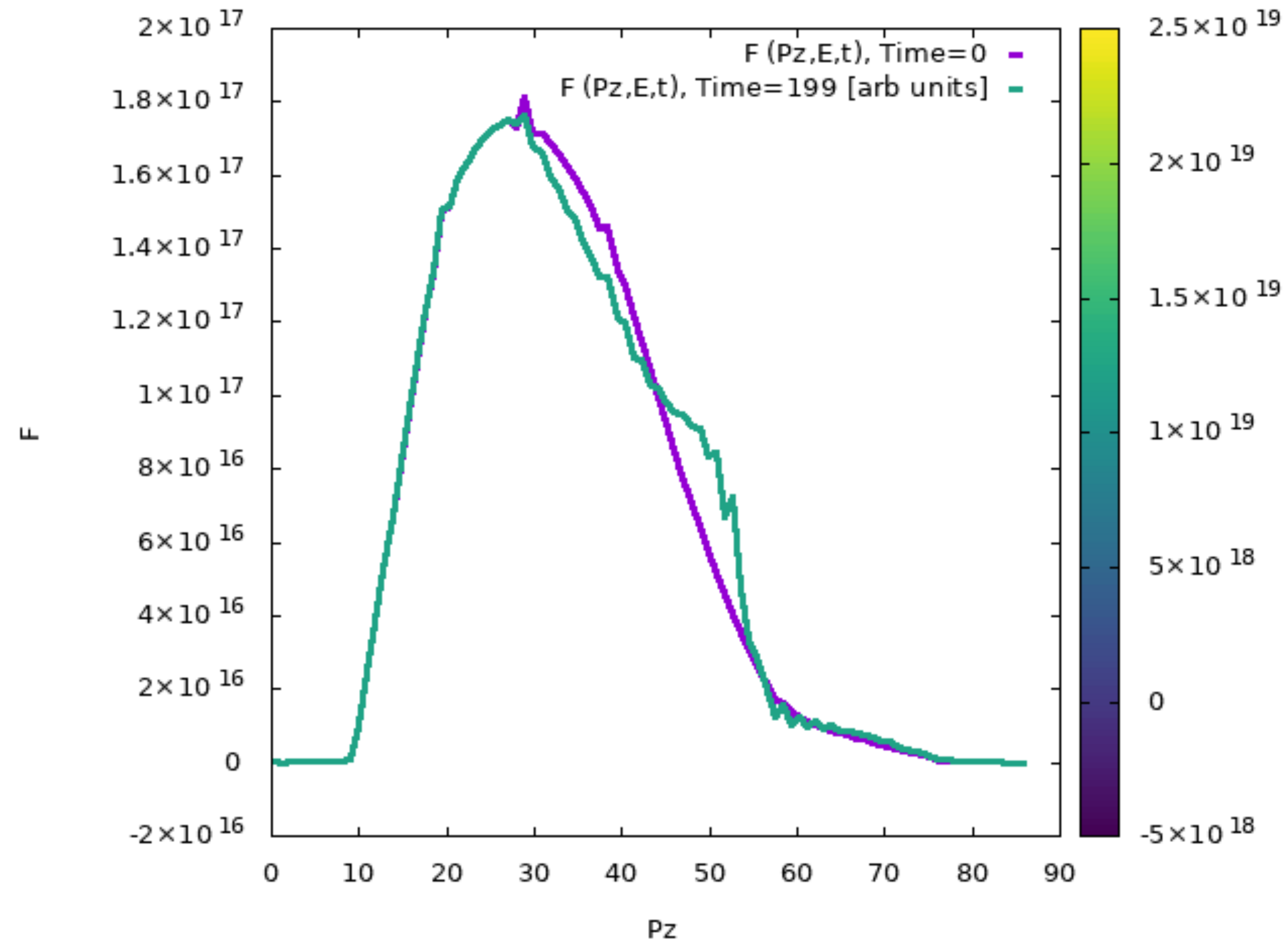
$F(t) - F(t=0)$, Time=147 [arb units]



$F(t) - F(t-1)$, Time=2 [arb units]

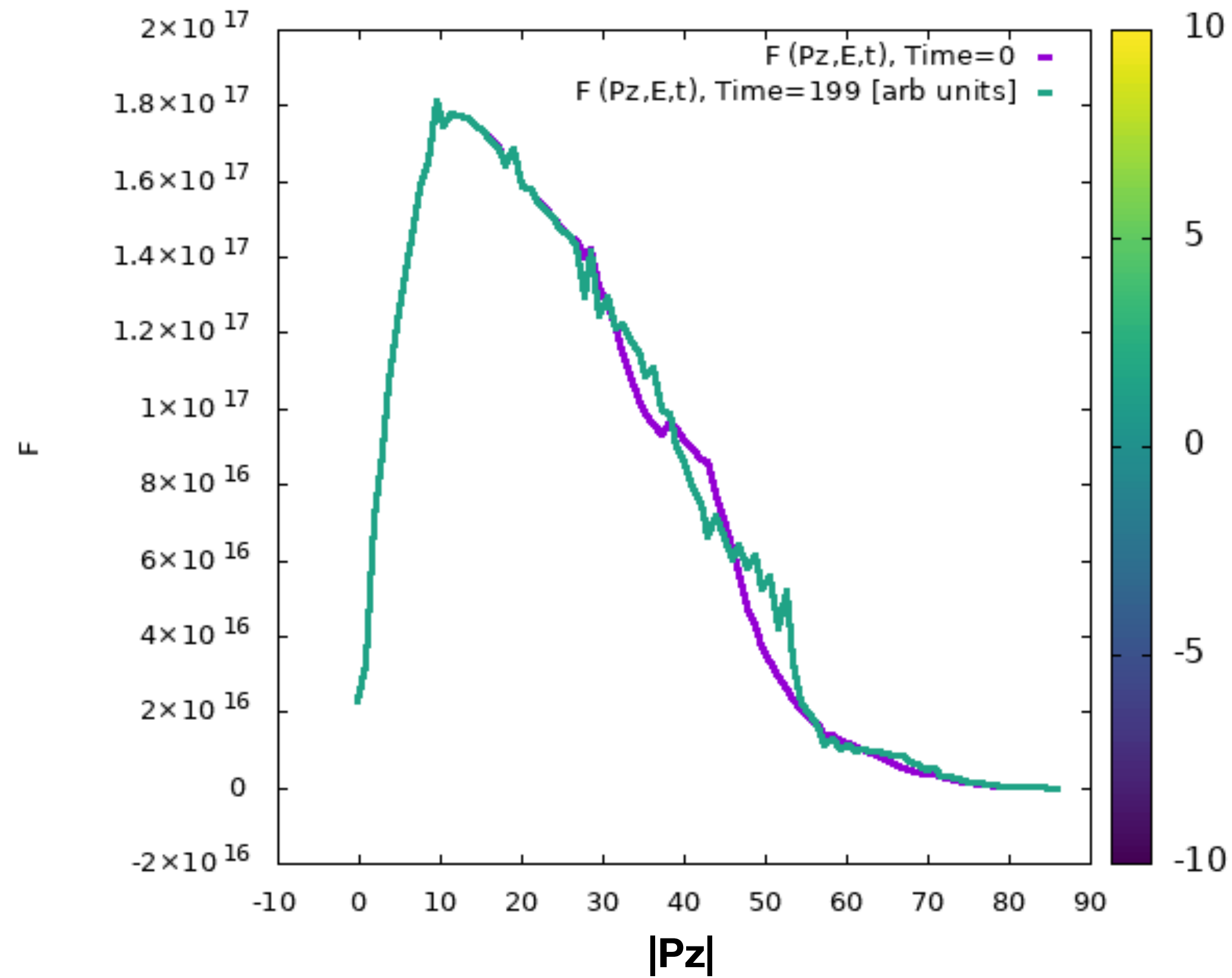


- secondary fine-structures start to evolve, as expected: in kick-model limit, amplitude is not changed - in real system amplitude would decay when gradients are exhausted
- source (RABBIT) and collisions models are currently implemented in ATEP code (G. Meng) - will smooth emerging steep gradients

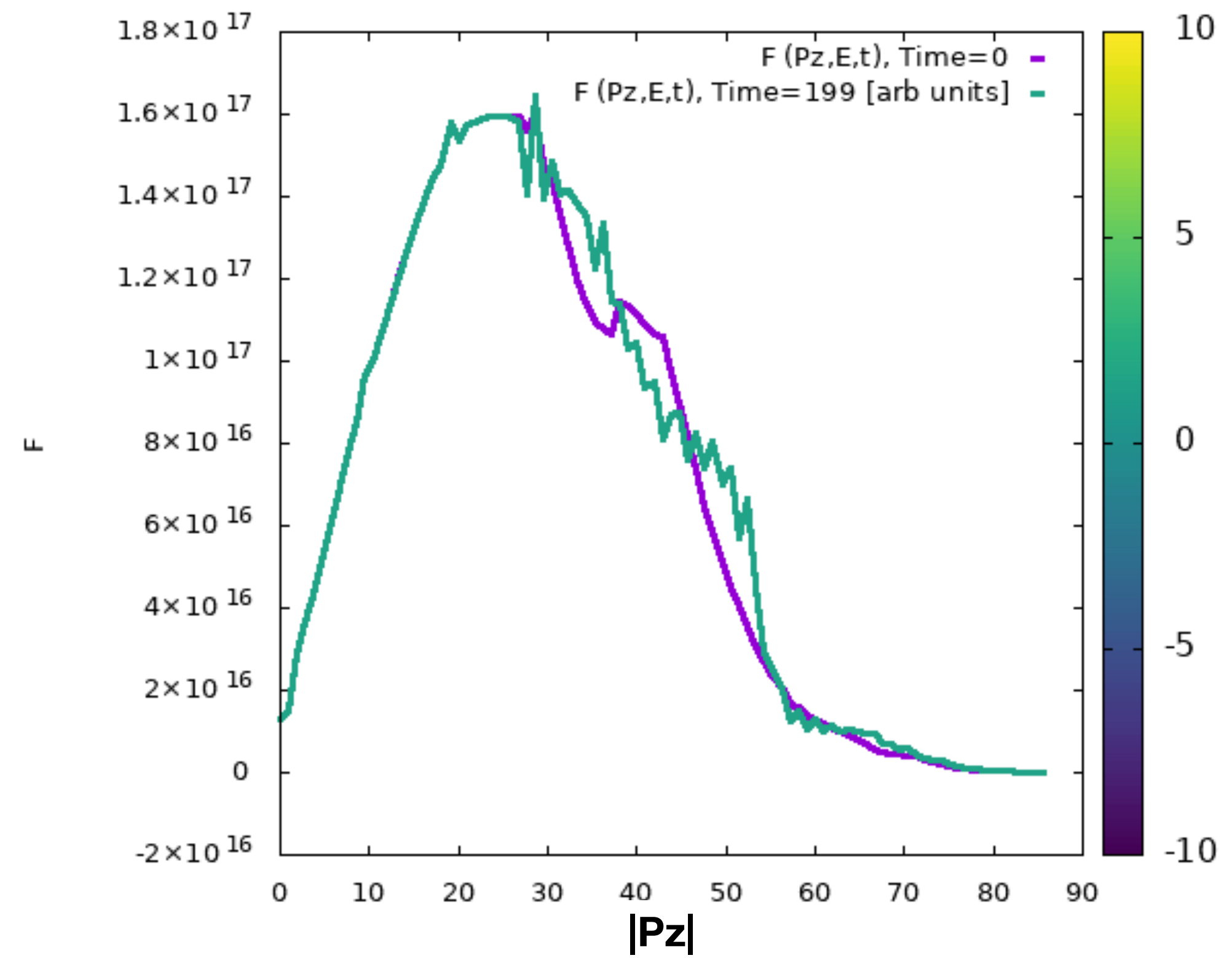


using ITER NBI off-off configuration

$|P_z|$

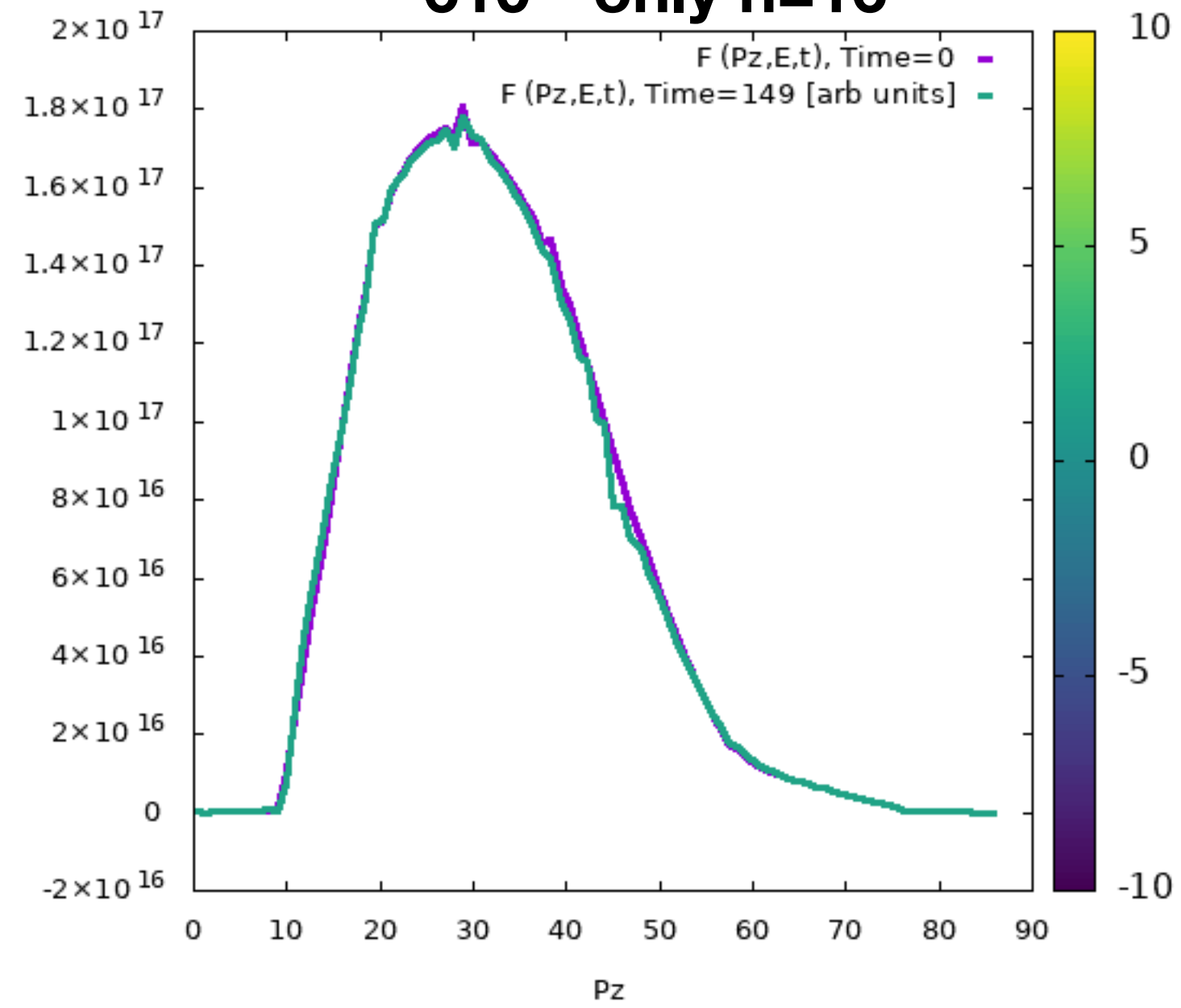


using ITER NBI on-on configuration

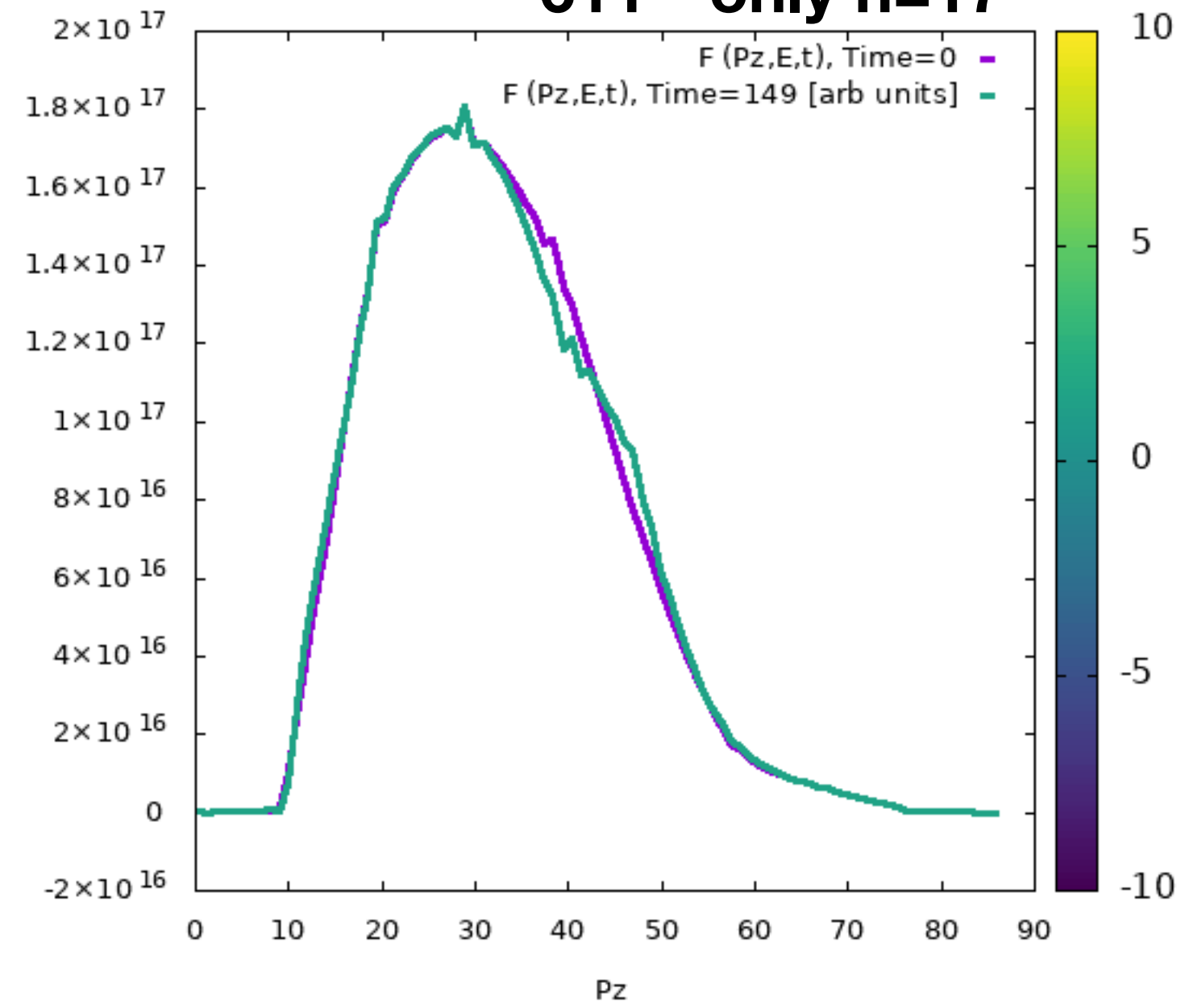


using ITER NBI on-off configuration

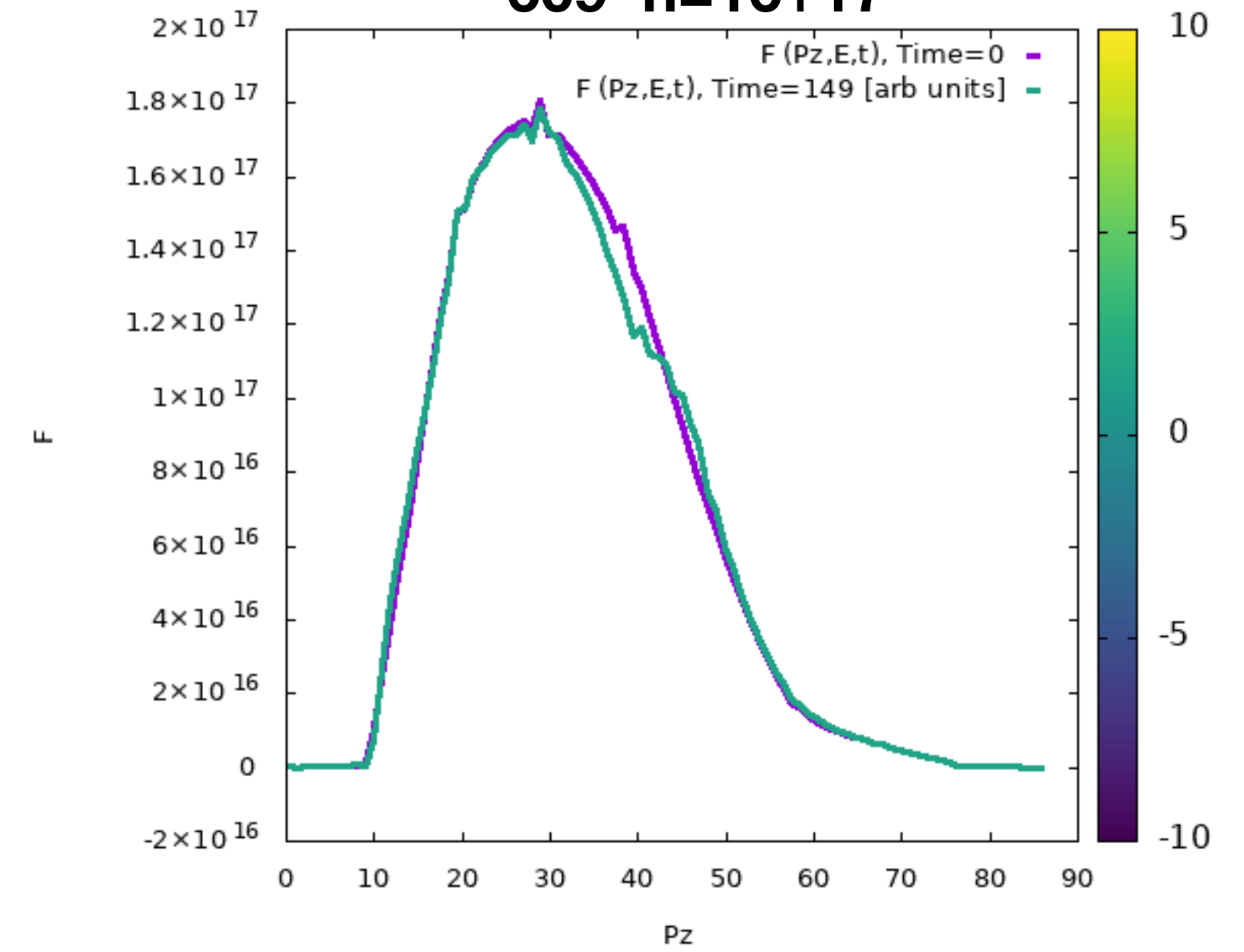
610 - only n=16



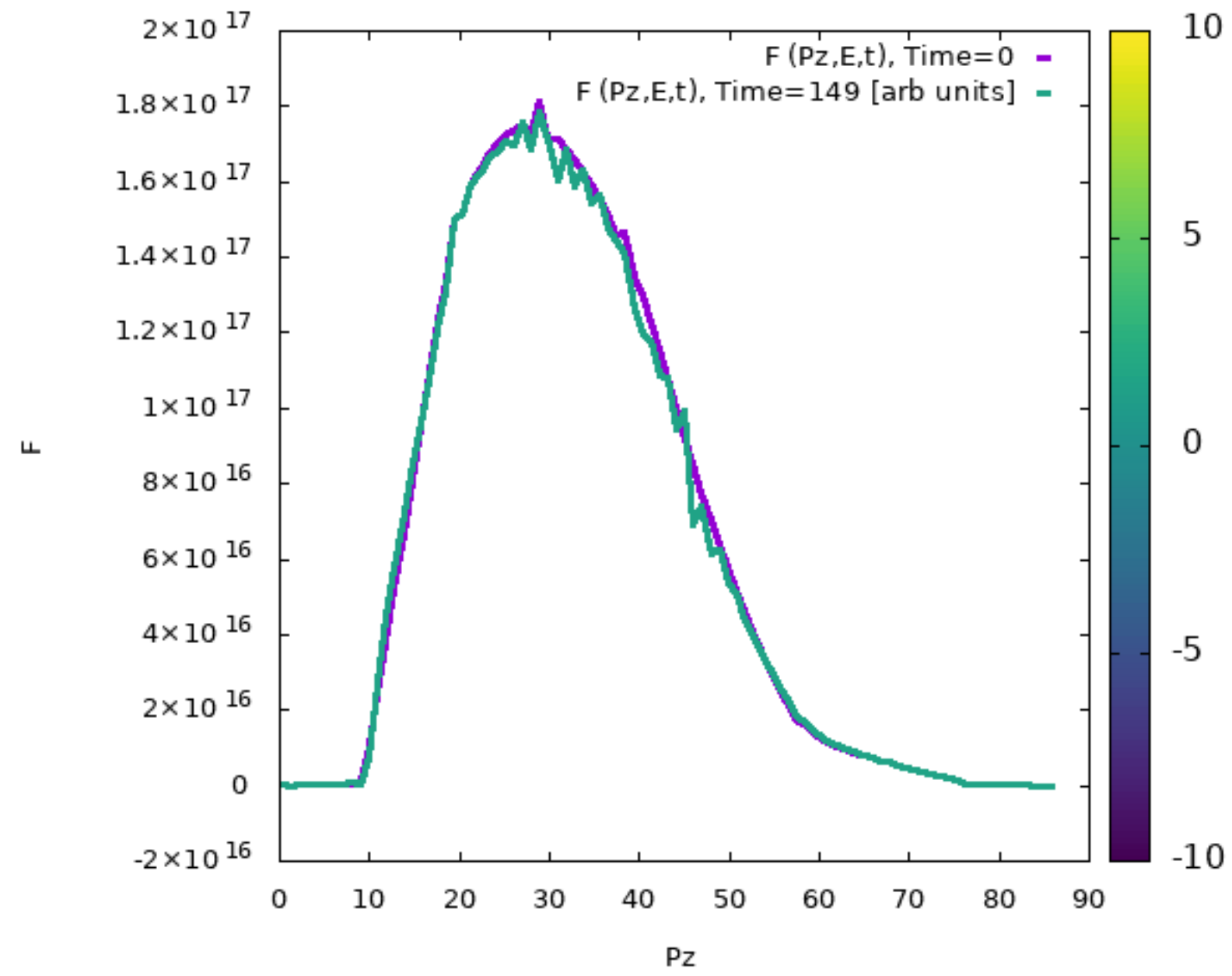
611 - only n=17



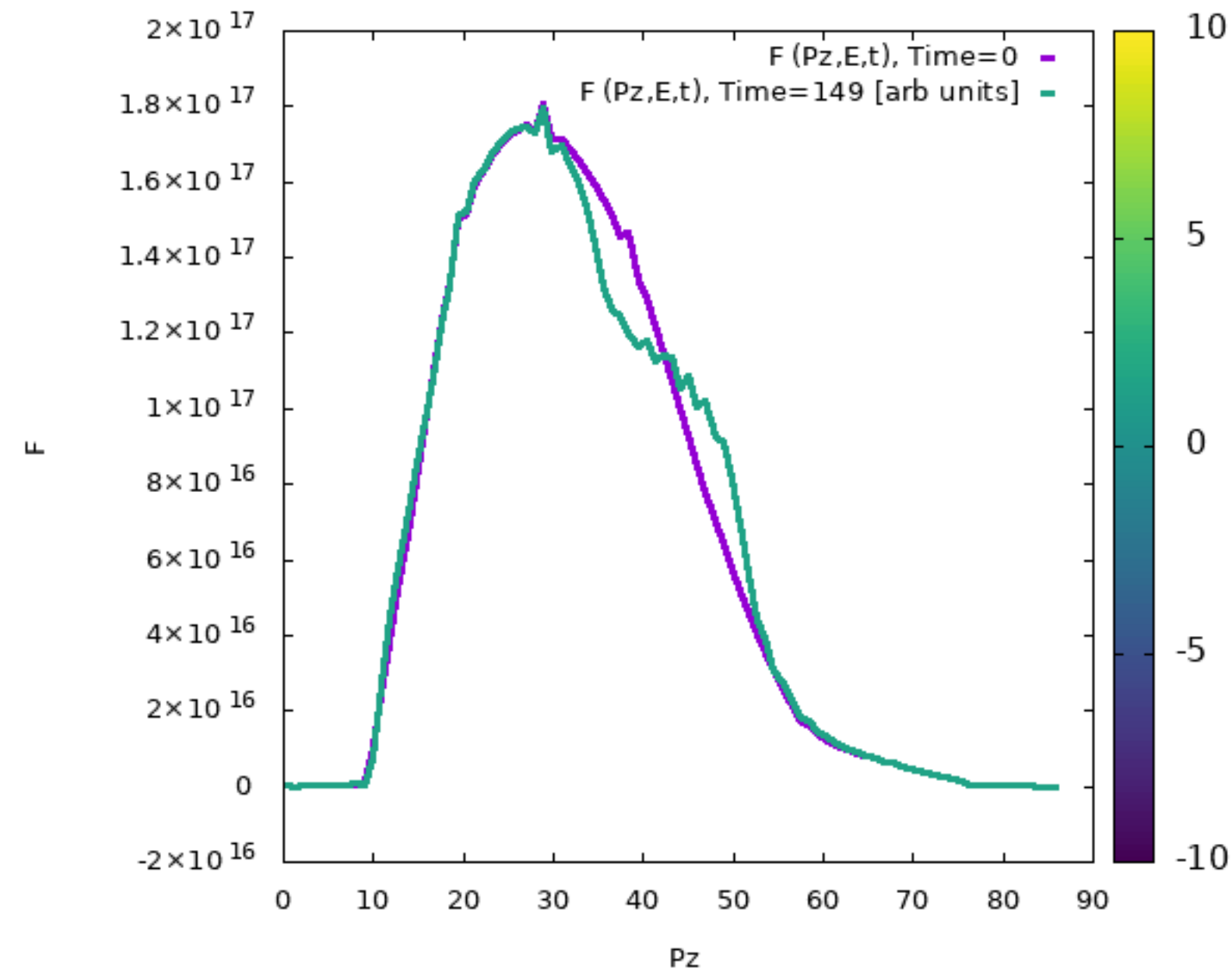
609 n=16+17



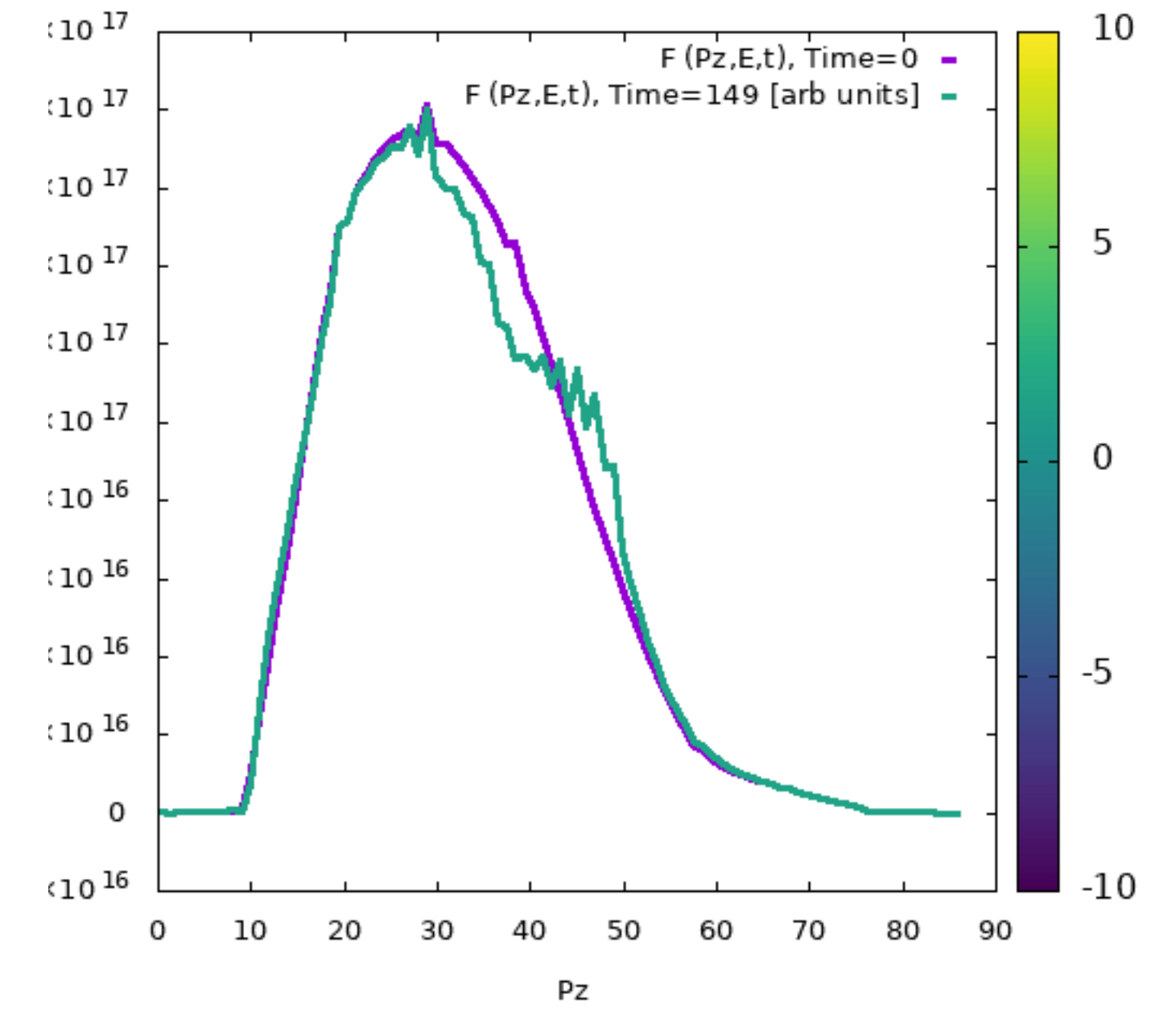
603 - only n=16



605 - only n=17



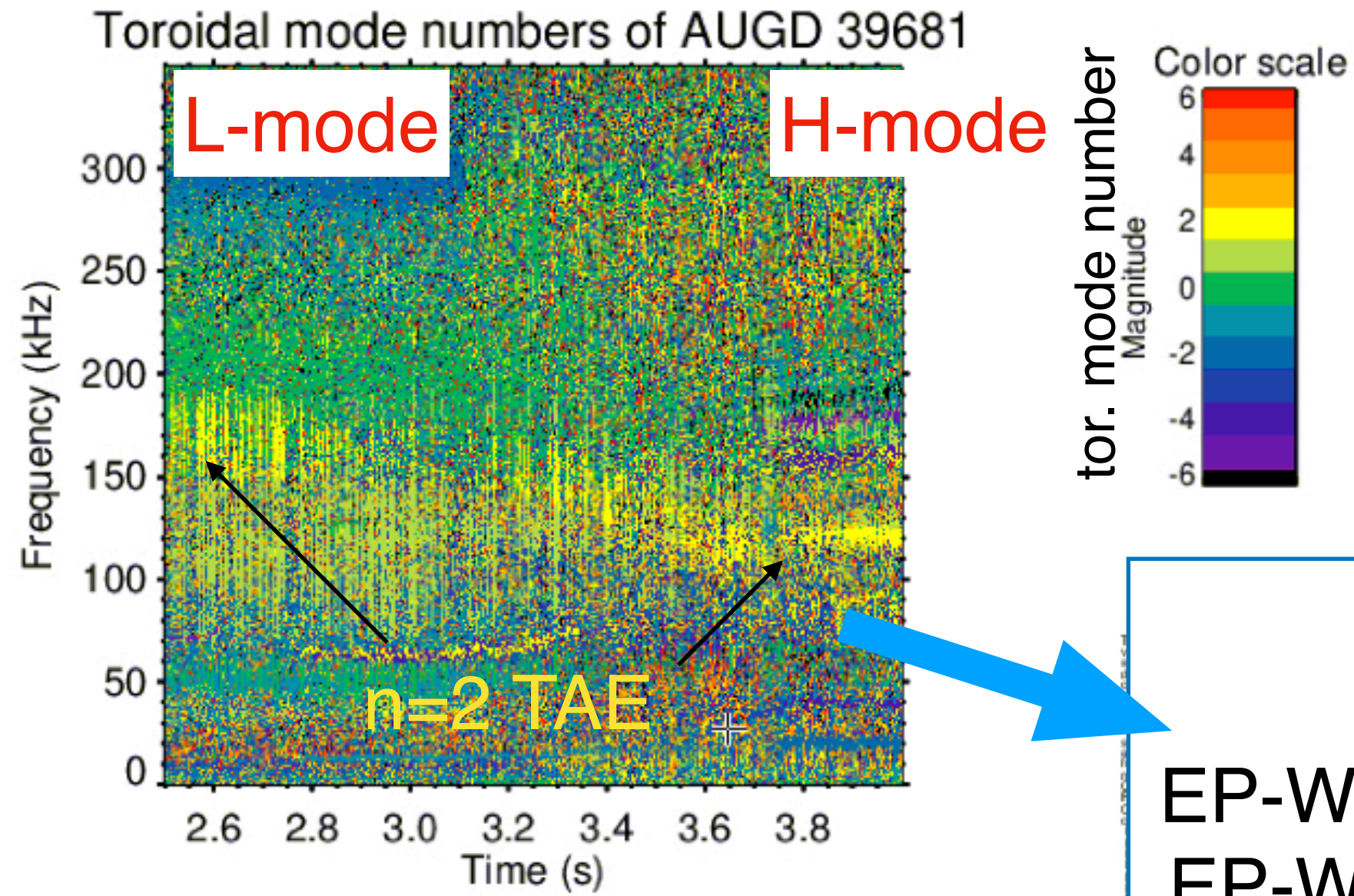
604 n=16+17





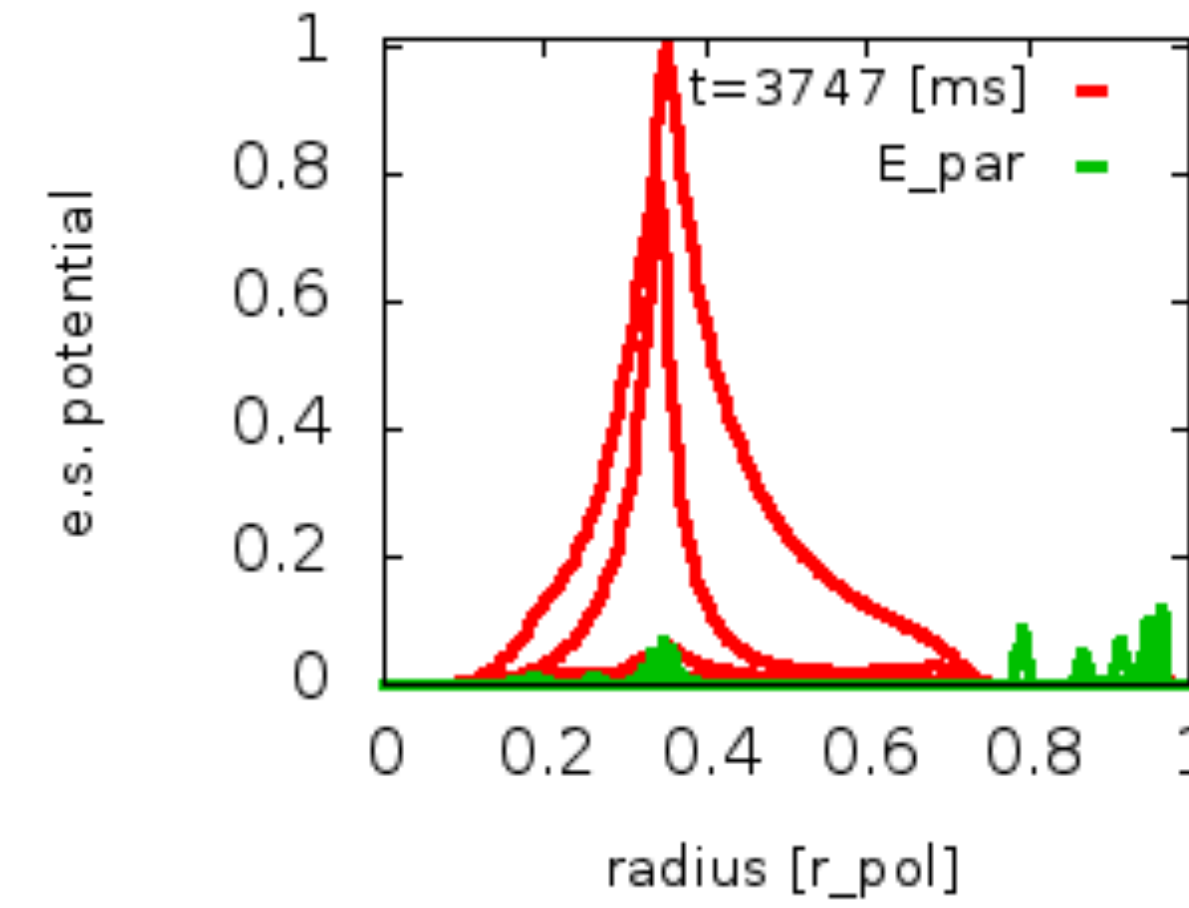
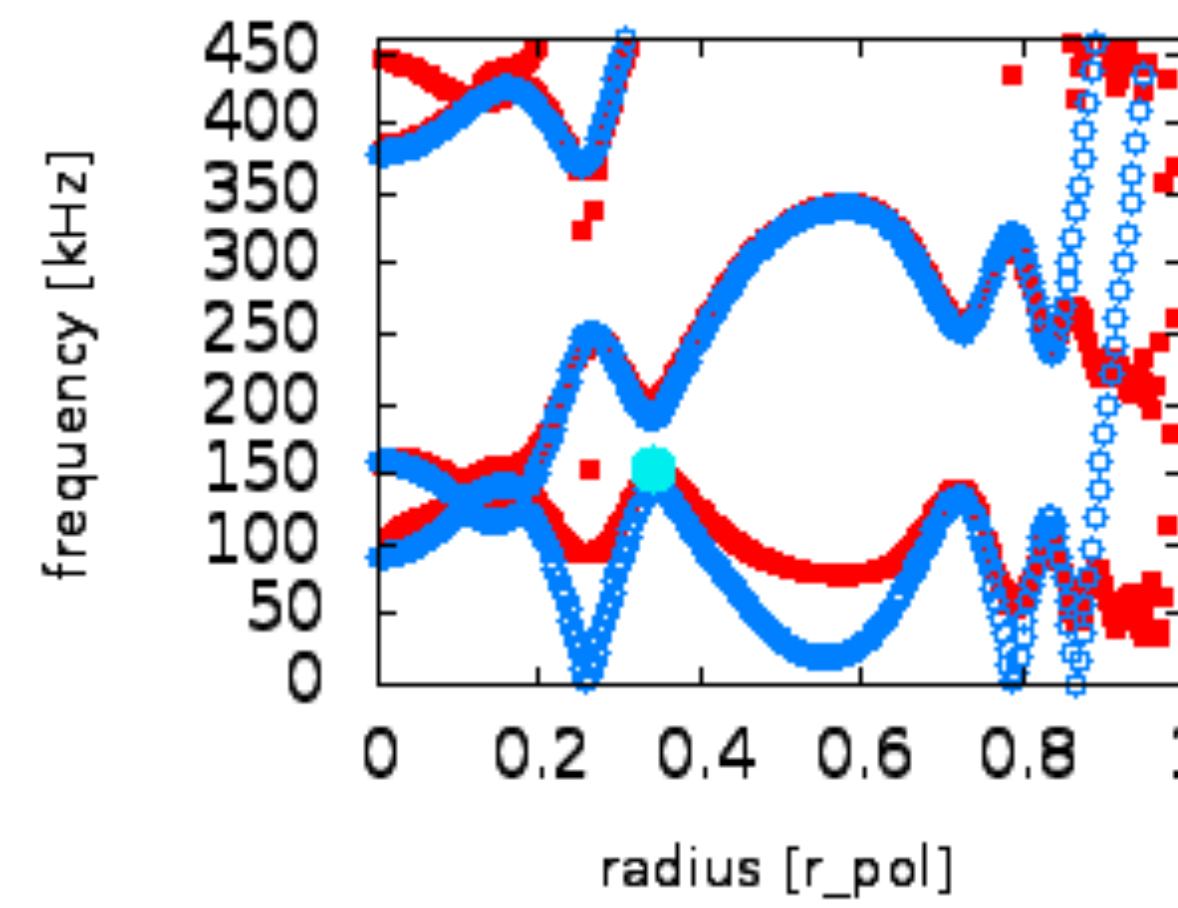
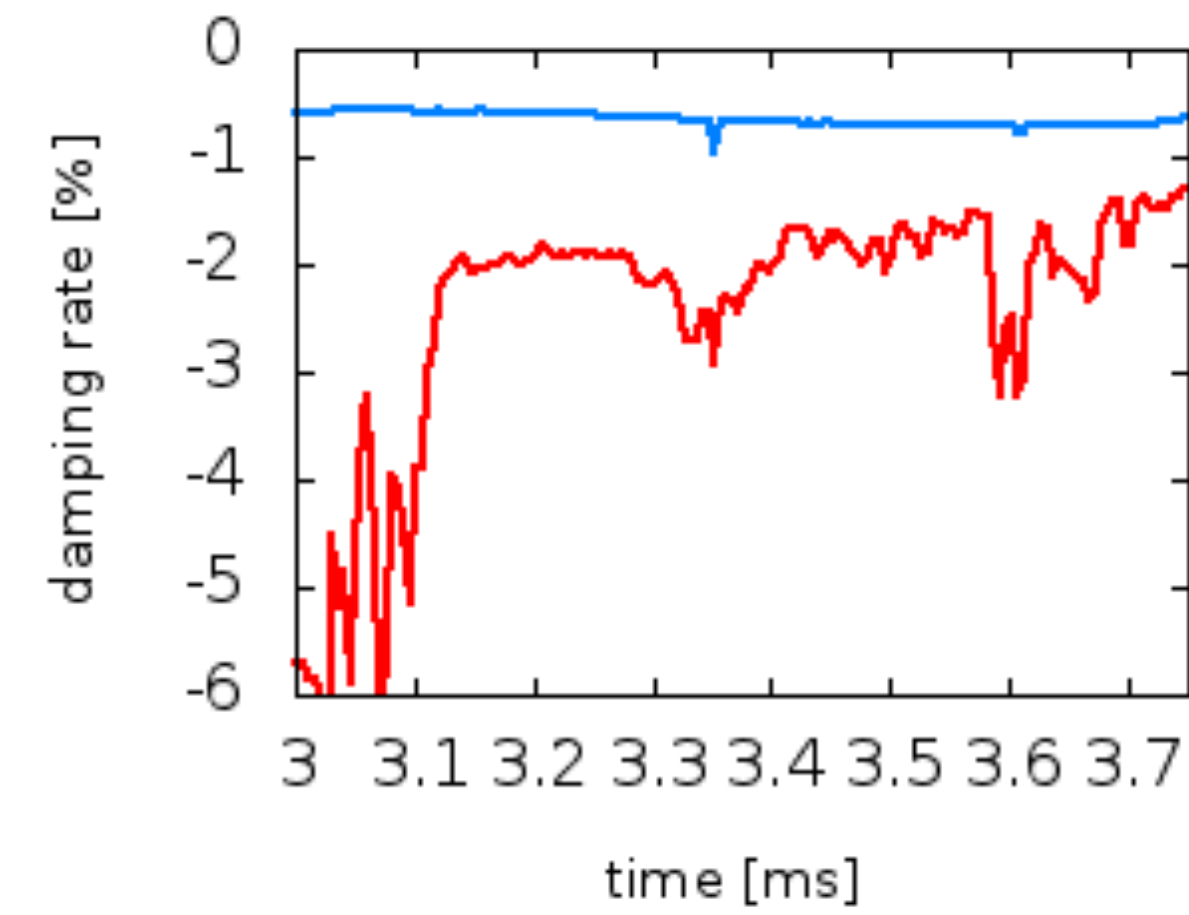
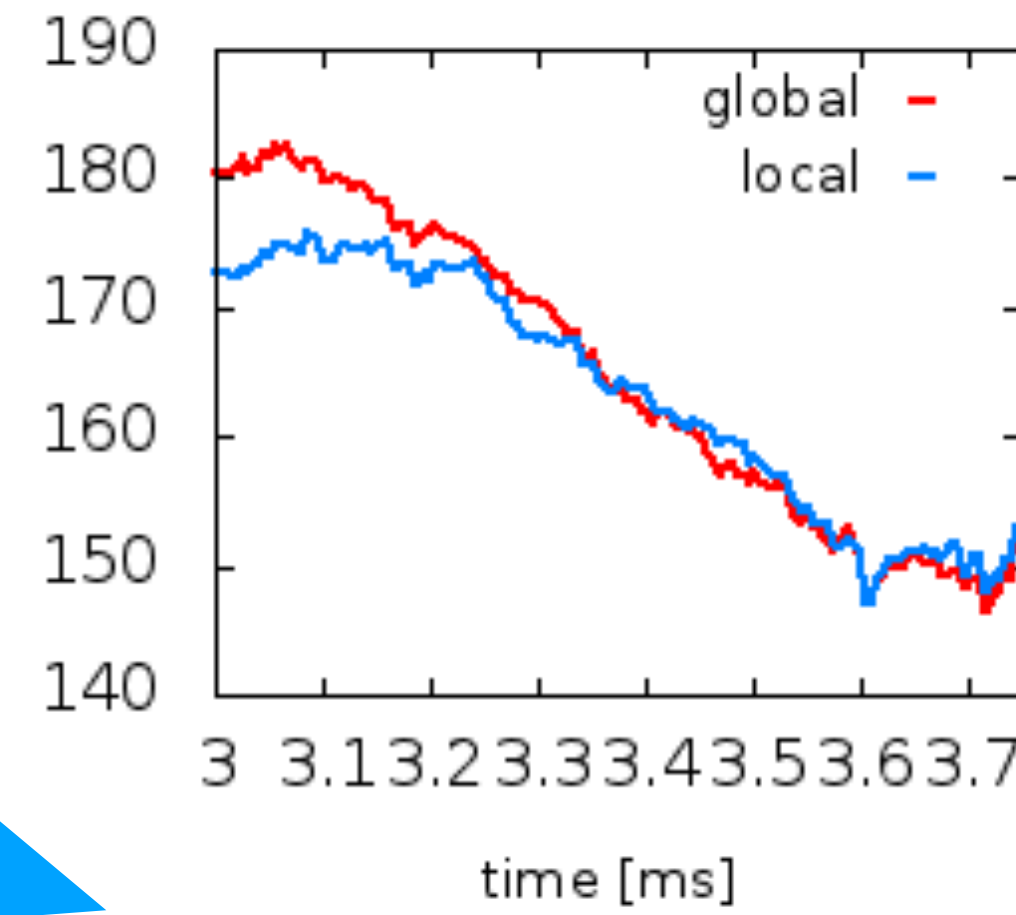
validation plans

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

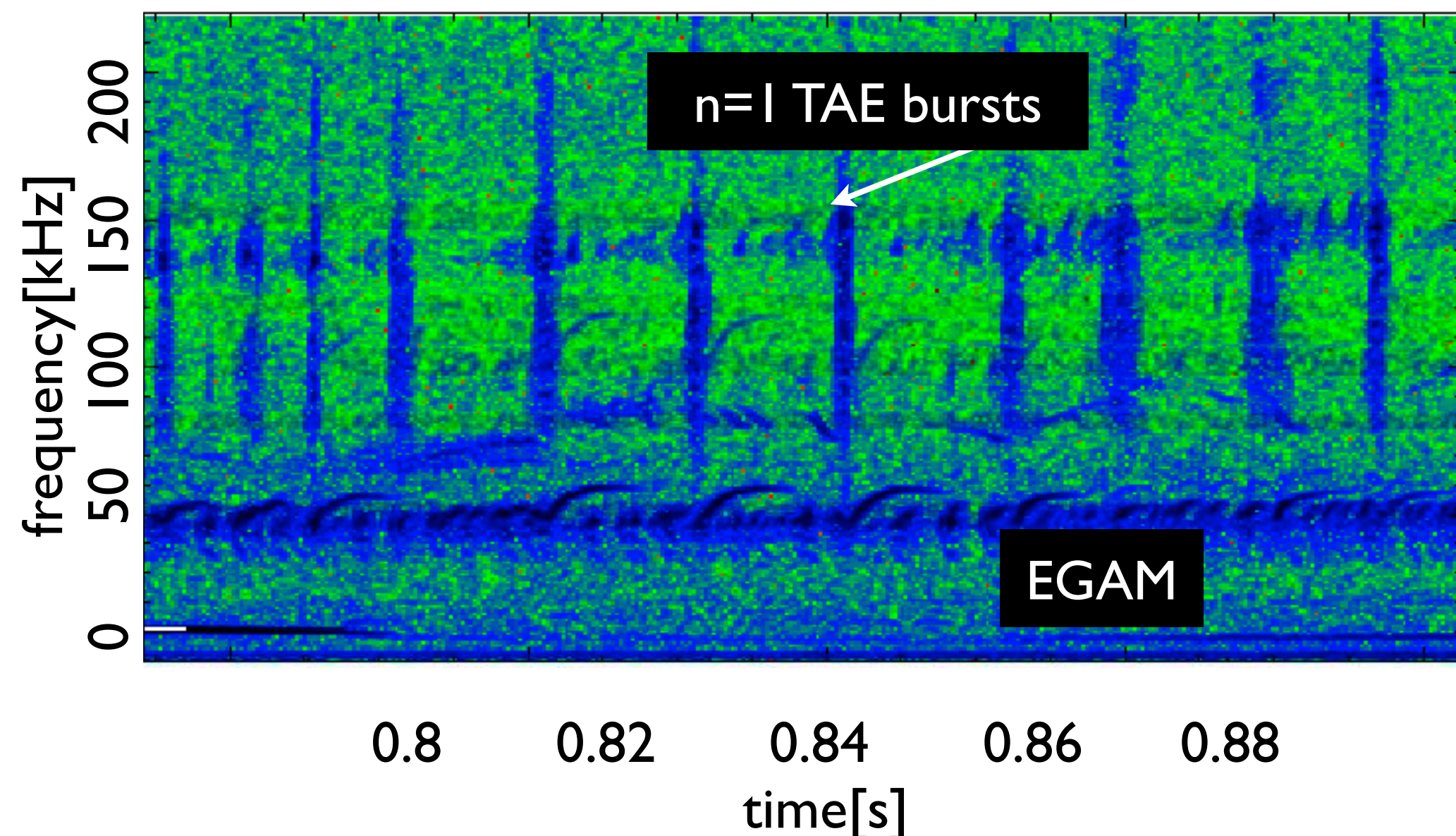


IDA +
TRVIEW +
EP-WF: LIGKA local +
EP-WF: LIGKA global

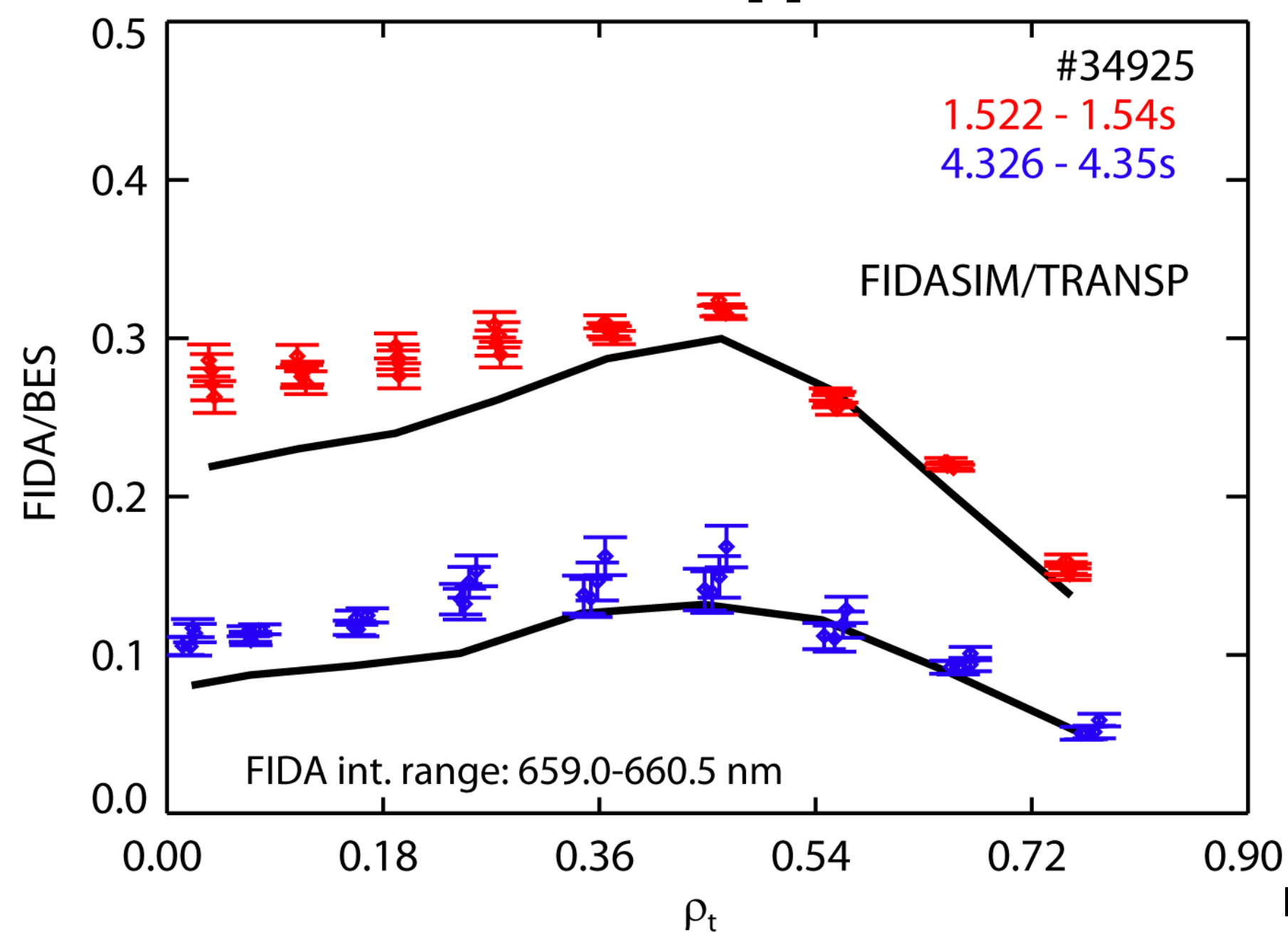
- automated processing of 160 time slices based on IDA equilibria and profiles
- fully implemented in IMAS, ensuring reproducibility



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



- minimize ion and electron LD by:
- cold core plasma despite strong EP drive (NBI)
- let impurities accumulate in core, heat only off-axis
- EP pressure dominated plasma - very useful for validation [benchmark paper Vlad et al NF 2021, and at this workshop] of non-linear physics
- reaches for EP physics relevant parameters:
 $\beta_{EP}/\beta_{thermal} \sim 1, E_{NBI}/T_{i,e} \approx 100$



- off-axis peaked EP profile
- modes are driven by negative and positive EP gradients
- measurable inwards EP transport with charge-exchange measurements

L. Horvath et al, Nucl. Fusion 56, 112003 (2016) [link](#)

Ph. Lauber et al, 27th IAEA FEC (2018) [link](#)

A. Di Siena, et al, Nucl. Fusion 58, 106014 (2018) [link](#)

I. Novikau, et al, accepted for publication in Comput. Phys. Commun. (2019) [arXiv](#)

F. Vannini, et al, Phys. Plasmas 27, 042501 (2020) [arXiv](#) - [link](#)

F. Vannini, et al, Physics of Plasmas 28, 072504 (2021)- [link](#)

I. Novikau, et al, Phys. Plasmas 27, 042512 (2020) [link](#)

M. V. Falessi, et al, J. Plasma Phys. (2020) [link](#)

Ph. Lauber et al, 28th IAEA FEC (2020) [link](#)

G. Vlad et al 2021 Nucl. Fusion 61 116026 [link](#)

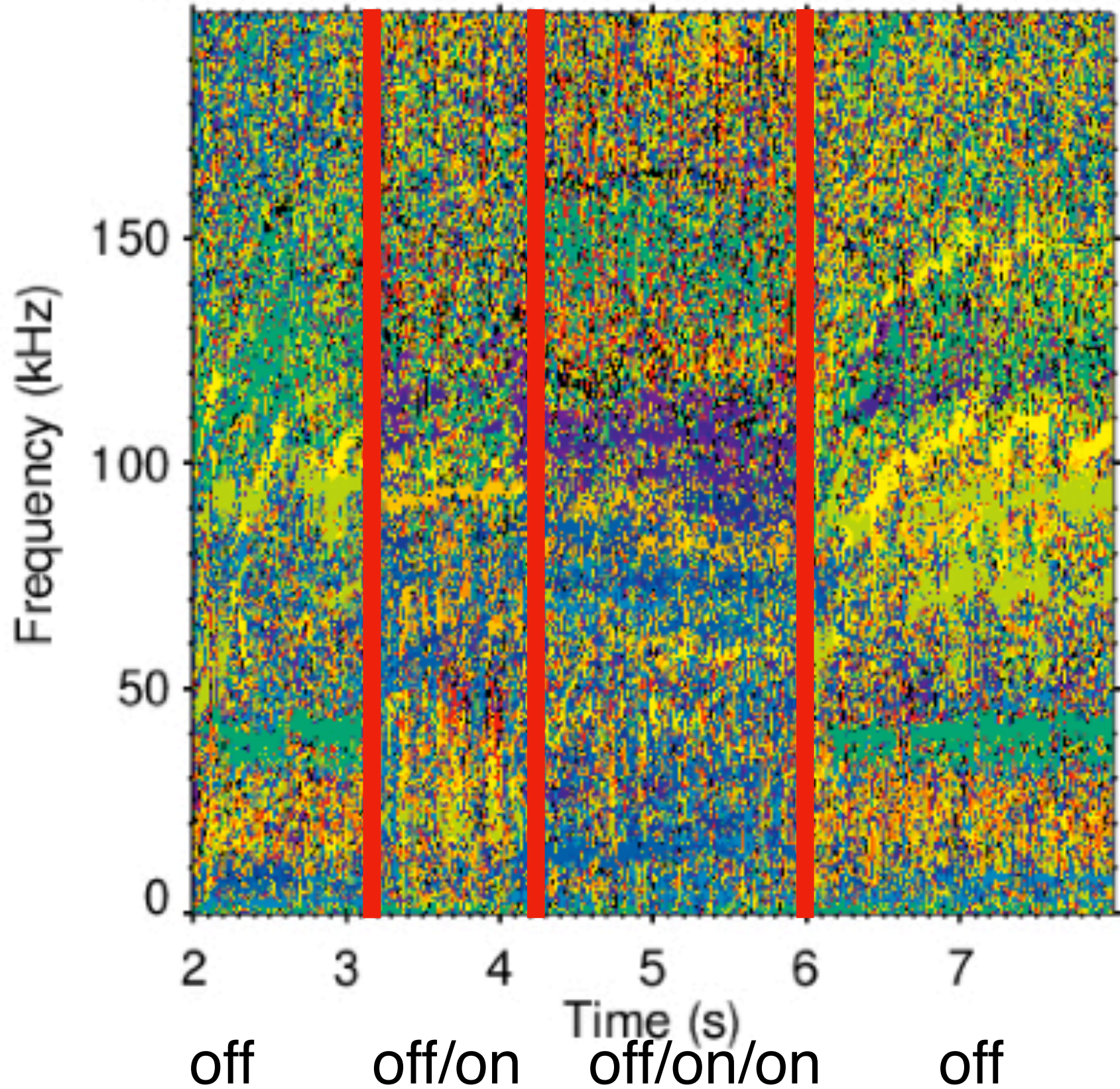
B. Rettino, 2022 Nucl. Fusion 62 076027

F. Vannini 2022 Nucl. Fusion 2022 accepted

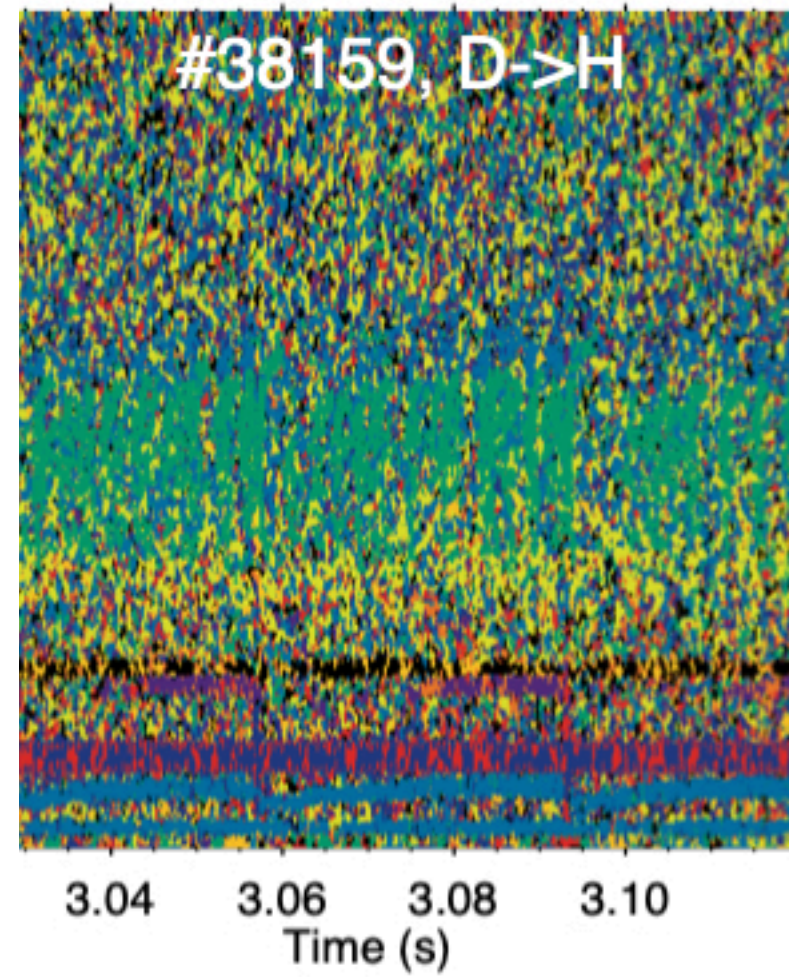
- exhaustive data for FOW/FLR effect studies
- higher L-H transition threshold in H allows for improved profile measurements in L-mode
- various combinations of on and off-axis beams with modes propagating in both electron and ion diamagnetic directions
- non-linear mode-mode interaction documented via bi-coherence analysis [Lauber FEC 2018]

helium plasma, D beams

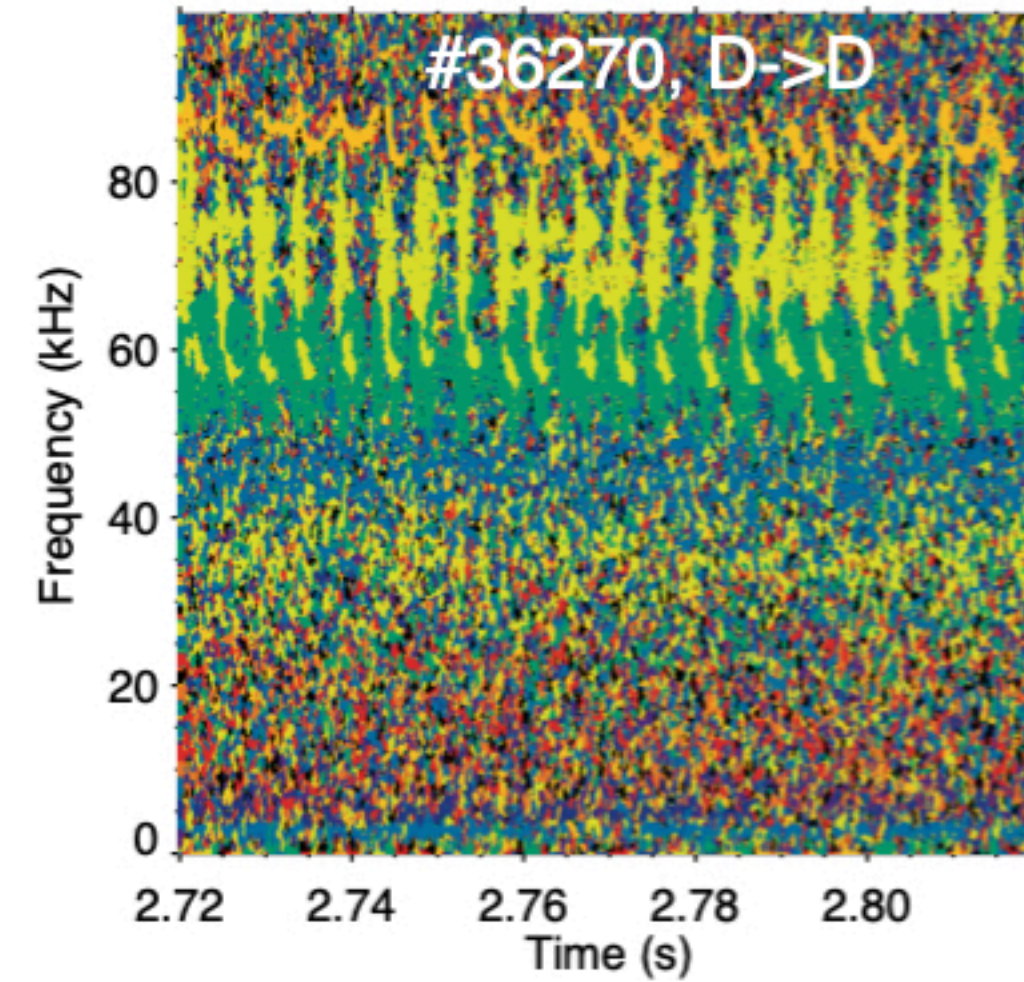
Toroidal mode numbers of AUGD 41437



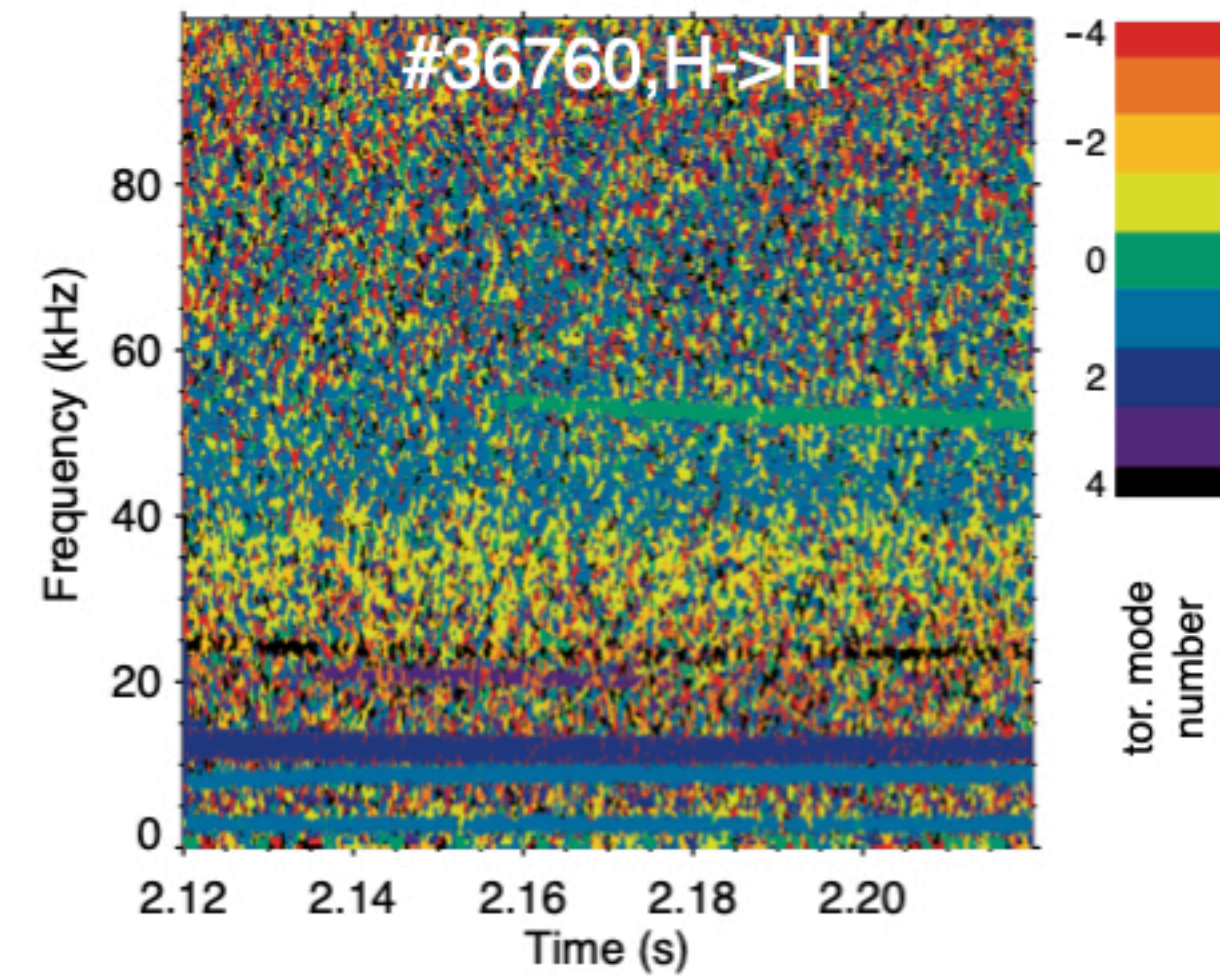
hydrogen plasma, D beams



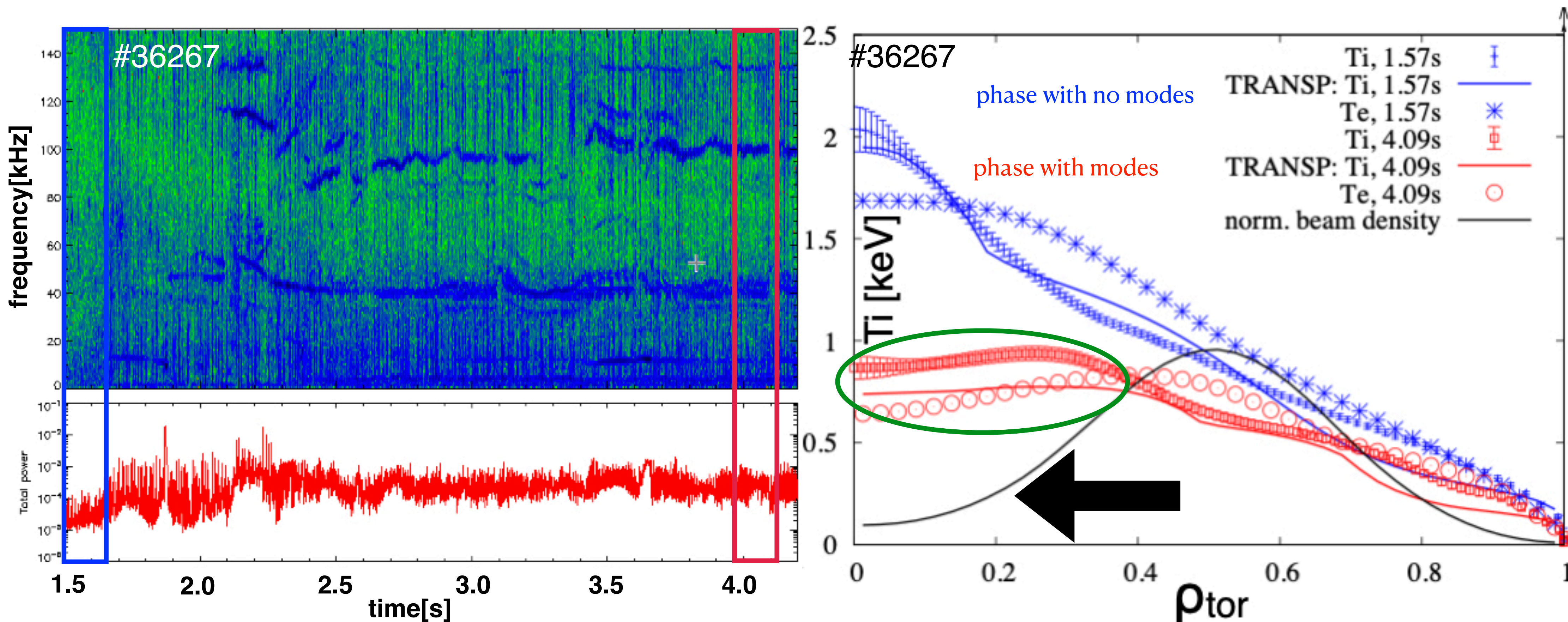
deuterium plasma, D beams



hydrogen plasma, H beams



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



other cases/experiments very welcome - TCV, JET, JT-60SA, ITER ongoing

summary & outlook

- IMAS-based PSZS transport model has been setup via coupling linear GK and non-linear drift-kinetic codes
- general F_{EP} generated from 'neoclassical' marker data can be used
- evolved PSZS transport equation in COM space in kick-model limit - mapping to real space available
- dedicated experiments at AUG address strongly non-linear EP regimes and diagnose related EP transport

next steps:

- calculate $D(s,E)$ - couple to RABBIT/transport codes
- add amplitude dependence of PSZS i.e. $d(dP/dt)dPz * F_{EP}$ term -> similar to RBQ model
- add various intensity closure models - analytical theory/ORB5/...
- add collisions and sources - bounce averaged collision operators - compare with models/codes e.g. CKA-EUTERPE [Brizard, Slaby/Kleiber, Hoppe,...]
- check diffusive vs convective cases, different mode spectra, overlap criteria
- separate scales according to PSZS theory → use to evolve to non-linear equilibria
- include (PS)ZSs due to turbulence, explore interaction in various limits

- speed up, hopefully export support next year via Eurofusion, integrate in workflow framework