WP 2.2

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common ‘ingredients’ of transport models:

- dispersion relation
- linear mode structures (parallel, radial)
- linear growth/damping rates
- orbit/zonal averages over mode structures
- nl evolution/ saturation amplitudes
- …

depend on:
equilibrium
kinetic profiles
distribution

can be calculated
with different fidelity vs speed

(i) the solution of the linearized Eqs. (2) and (3); (ii) the solution of the NLSE-like equation for the nonlinear envelope equations, Eq. (10); (iii) the solution of Eqs. (20), (23) and (25) for the particle response averaged over linear parallel mode structures.

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improvements/extensions of LIGKA are subject of WP 2.2

milestones of WP 2.2

WP2.2-M1: Develop (semi-)analytical trapped particle model for LIGKA: end 2022

WP2.2-M2: Test and tune analytical global mode structure model for LIGKA/HAGIS end 2022

WP2.2-M3: Generalize fast analytical LIGKA version to non-Maxwellian distribution functions, in particular slowing down end 2023

WP2.2-M1: trapped particles:

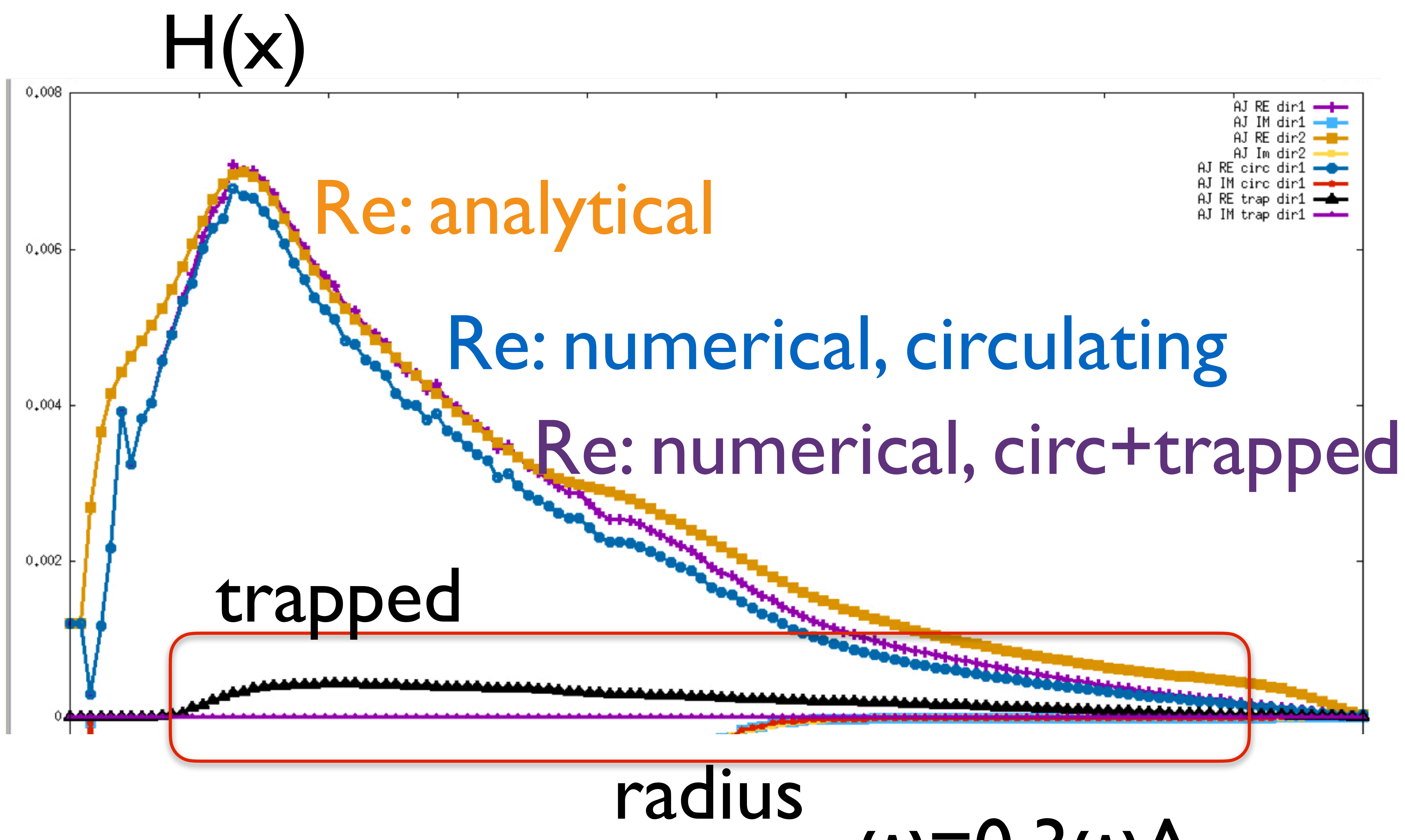
$$\sum_m \omega^2\left(1-\frac{\omega_{*p}}{\omega}\right) - k_\parallel^2\omega_A^2R_0^2 = 2\frac{v_{thi}^2}{R_0^2}\Bigg(-\Big[H(x_{m-1})+H(x_{m+1})\Big] + \tau\Big[\frac{N^m(x_{m-1})N^{m-1}(x_{m-1})}{D^{m-1}(x_{m-1})} + \frac{N^m(x_{m+1})N^{m+1}(x_{m+1})}{D^{m+1}(x_{m+1})}\Big]\Bigg)$$

[Zonca PPCF 1996,2009, Gotit lectures, Garbet 2006], [Lauber PPCF 2009]

circulating ion appoximation; extension trapped particles [I. Chavdarovski et al, 2014…]

$$h = -e_a \sum_m \sum_k \underbrace{\frac{\frac{\partial F_0}{\partial E}(\omega-\hat{\omega}_*)e^{-im\theta}J_0}{(\omega-\omega_D^0 - H\sigma S_m^0\omega_t - k\omega_{b,t})}}_{=\mathcal{R}_{m,k}}\left[a_{km}\phi_m(r) - (a_{km} - \frac{a_{km}^G\bar{\omega}_d(r)}{\omega})\psi_m(r)\right]$$

numerical results are available (LIGKA):



- which expression for barely/deeply trapped particles is most efficient?
- approximations for ωprec and ωb,t?
- which coordinates? map?
- when to be neglected? error?
- plans for DAEPS? Common module?

ω=0.3ωA

$$\sum_m \omega^2\Big(1-\frac{\omega_{*p}}{\omega}\Big) - k_\parallel^2\omega_A^2R_0^2 = 2\frac{v_{thi}^2}{R_0^2}\Bigg(-\Big[H(x_{m-1})+H(x_{m+1})\Big] + \tau\Big[\frac{N^m(x_{m-1})N^{m-1}(x_{m-1})}{D^{m-1}(x_{m-1})}+\frac{N^m(x_{m+1})N^{m+1}(x_{m+1})}{D^{m+1}(x_{m+1})}\Big]\Bigg)$$

[Zonca PPCF 1996,2009, Gotit lectures, Garbet 2006], [Lauber PPCF 2009]

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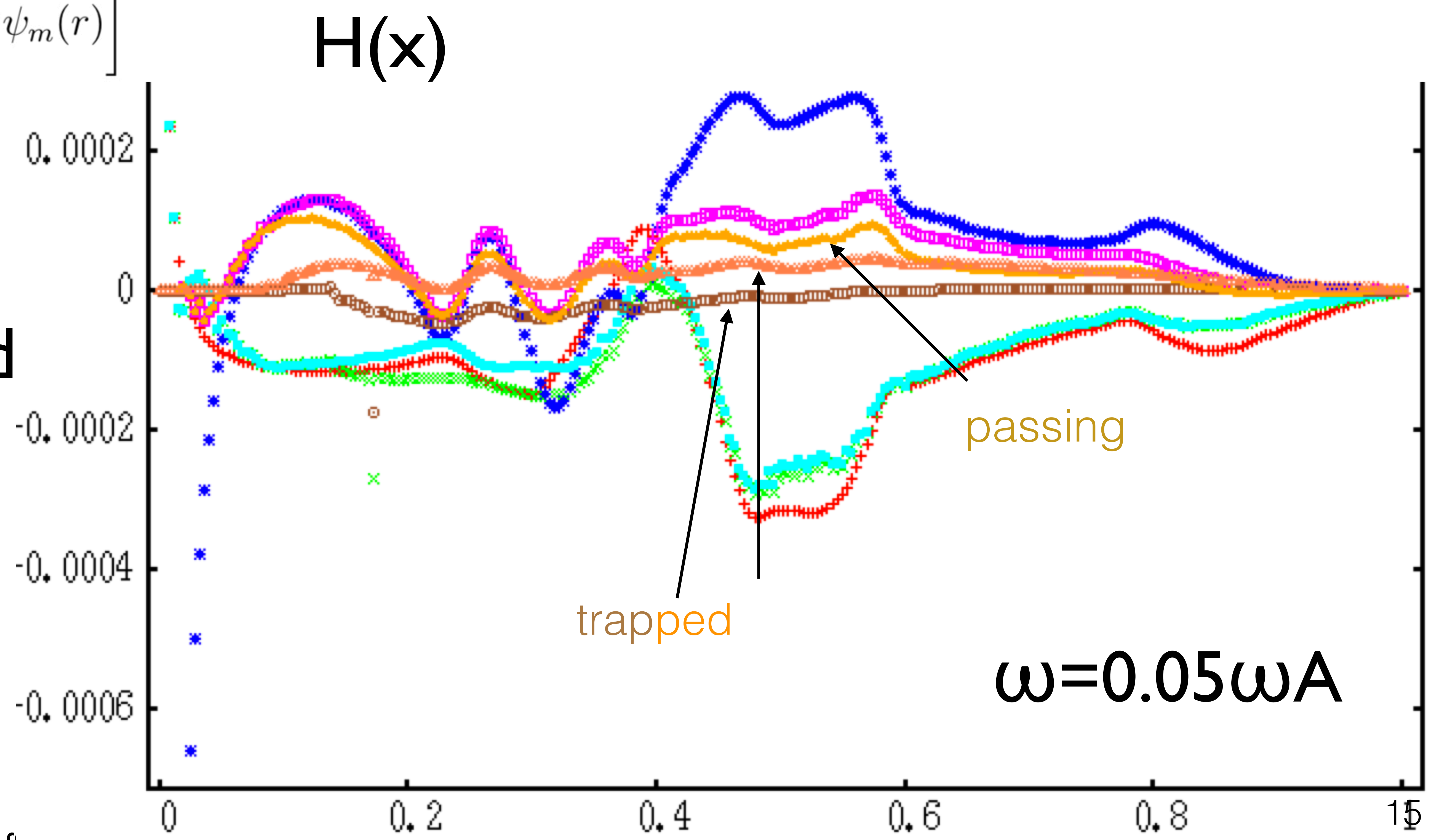
$$h = -e_a\sum_m\sum_k \underbrace{\frac{\frac{\partial F_0}{\partial E}(\omega-\hat{\omega}_*)e^{-im\theta}J_0}{(\omega-\omega_D^0-H\sigma S_m^0\omega_t-k\omega_{b,t})}}_{=\mathcal{R}_{m,k}}\Big[a_{km}\phi_m(r)-(a_{km}-\frac{a_{km}^G\bar{\omega}_d(r)}{\omega})\psi_m(r)\Big]$$

numerical results are available (LIGKA):

- which expression for barely/deeply trapped particles is most efficient?
- approximations for ωprec and ωb,t?
- which coordinates? map?
- when to be neglected? error? UQ?
- plans for DAEPS? Common module?



WP2.2-M2: estimate analytical mode structures:

[A. Popa]

motivation:

- analytical FLR and FOW expressions need kr - accurate value improves damping/growth rates
- decide, if local or global analysis for particular mode number is needed
- direct evaluation of kinetic integrals if e.g. Gaussians are assumed (Qualikiz)
- input can be used as initial conditions for initial value codes
- available literature on e.g. TAEs: depends on shear, alignment of gaps (radially/frequency); some twists when allowing odd/even coupling along the gap
- BAEs, RSAEs straightforward, also EAEs possible

test and verify for many scenarios/time points (WF-LIGKA)

WP2.2-M3: non-Maxwellian distribution functions

- extension to non-Maxwellian distribution functions according to [Hua-Sheng Xie, PoP 2013], bump-on-tail:

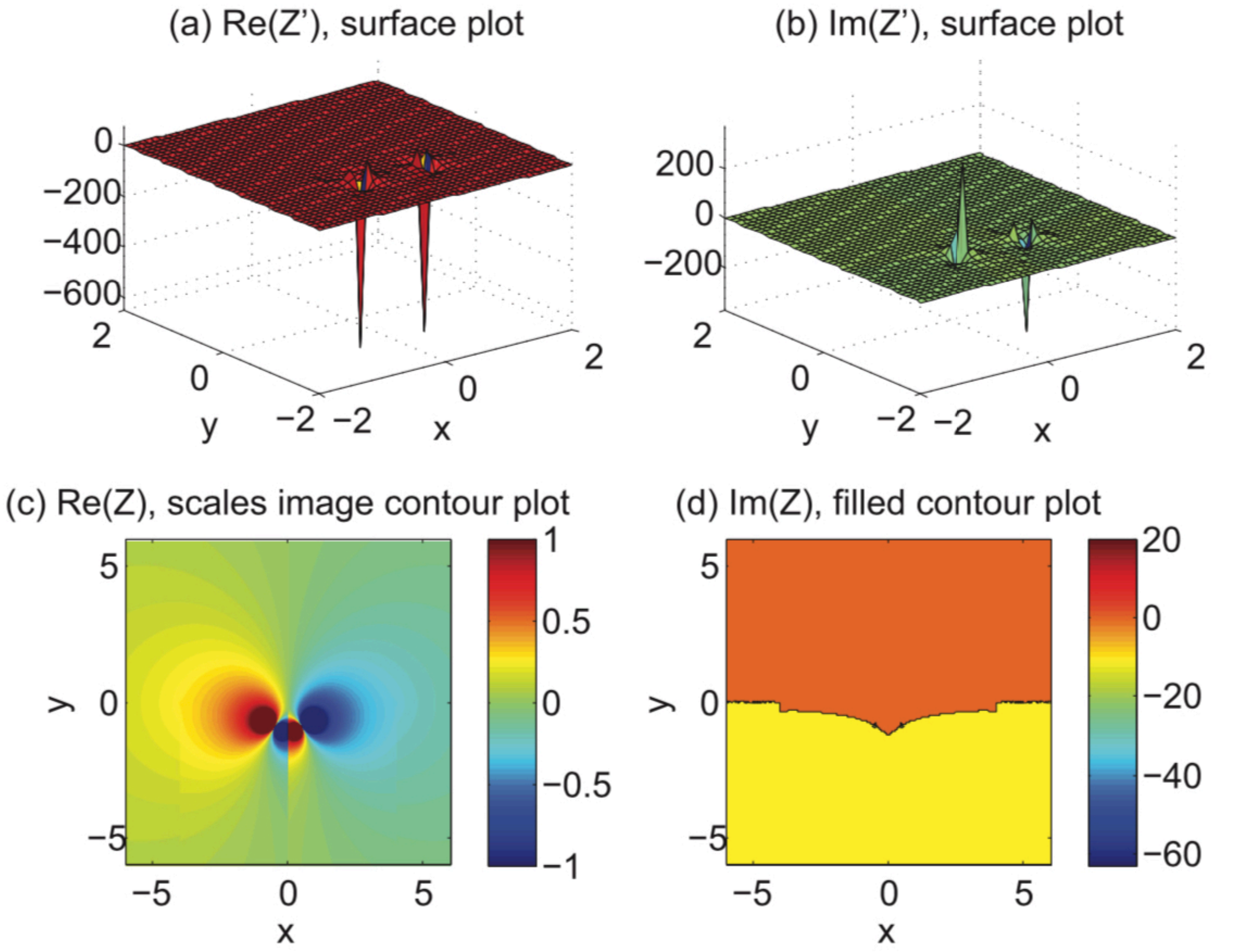
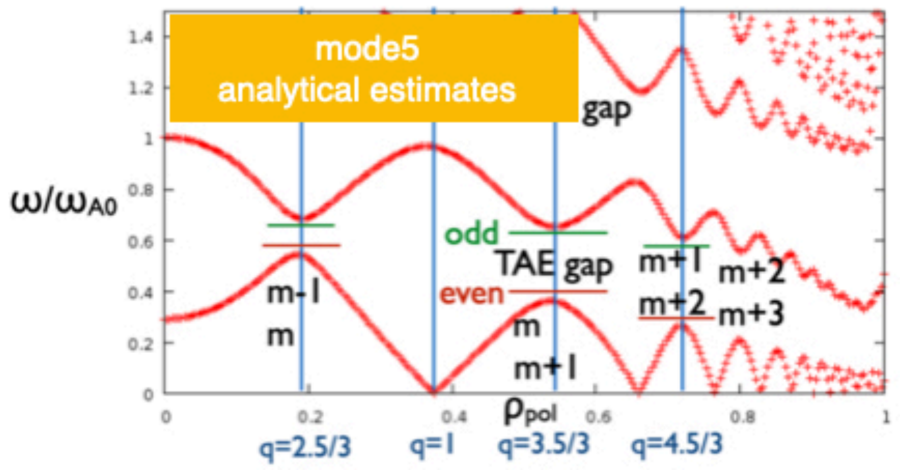


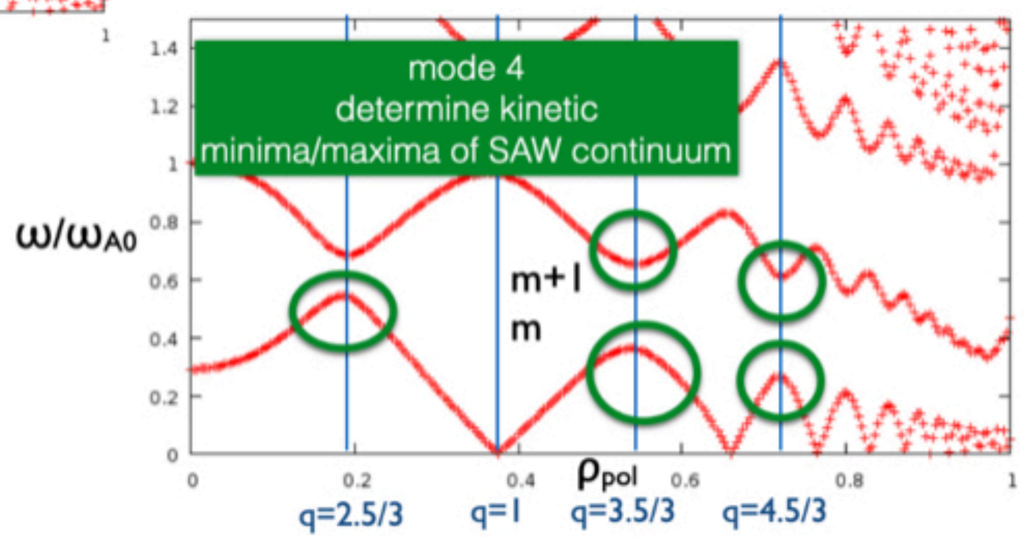
FIG. 10. Visualization of $Z(\zeta)$ and $Z'(\zeta)$ with input function F_{SD} for $v_t = 1$ and $v_c = 4$.

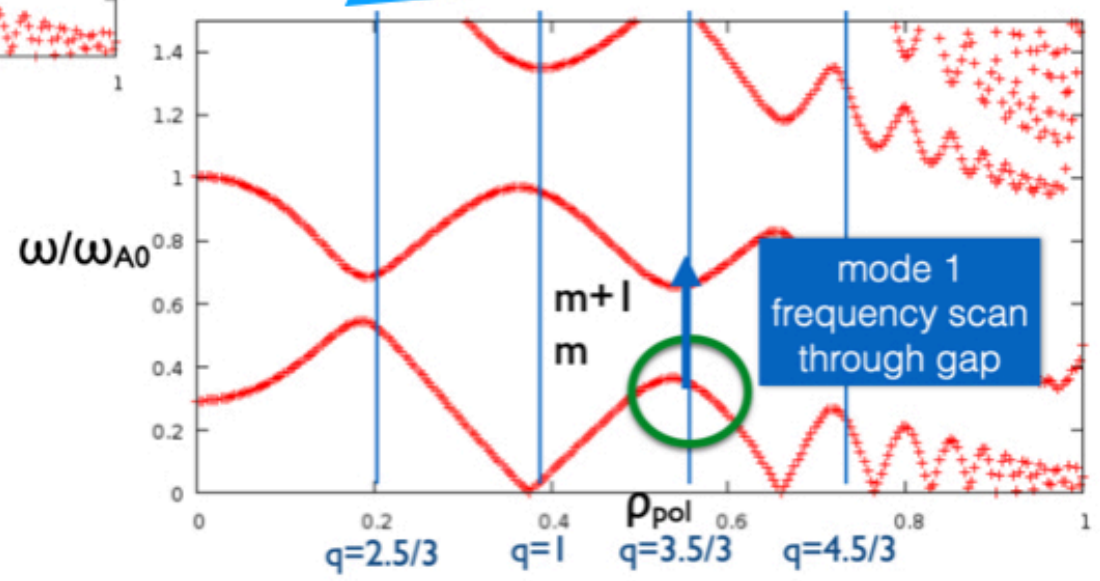
- Rabbit: can Legendre polynomial representation be exploited for (partial) analytical integration? (not COM, however…)
- LIGKA denominator is expanded in rational polynomials - analytical integration?

next steps:

- define a good test cases for benchmark/comparison with DAEPS
- define where shared development of model/implementation is possible
- test speed vs accuracy, UQ
- interface to transport models - IMAS updates/upgrades







mode5:
- [Fesenyuk 2014]
- [S.D. Pinches et al PPCF 2015)]
- suggestions for useful formulae can be easily implemented (LIGKA: sub_mode5.F)

WP 3.3

Ph. Lauber, Guo Meng, M. Weiland, A. Popa, M. Falessi

common ‘ingredients’ of transport models:

- dispersion relation
- linear mode structures (parallel, radial)
- linear growth/damping rates
- orbit/zonal averages over mode structures
- nl evolution/ saturation amplitudes
- calculate EP fluxes
- …

depend on:
equilibrium
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can be calculated
with different fidelity vs speed

Milestones WP 3.3

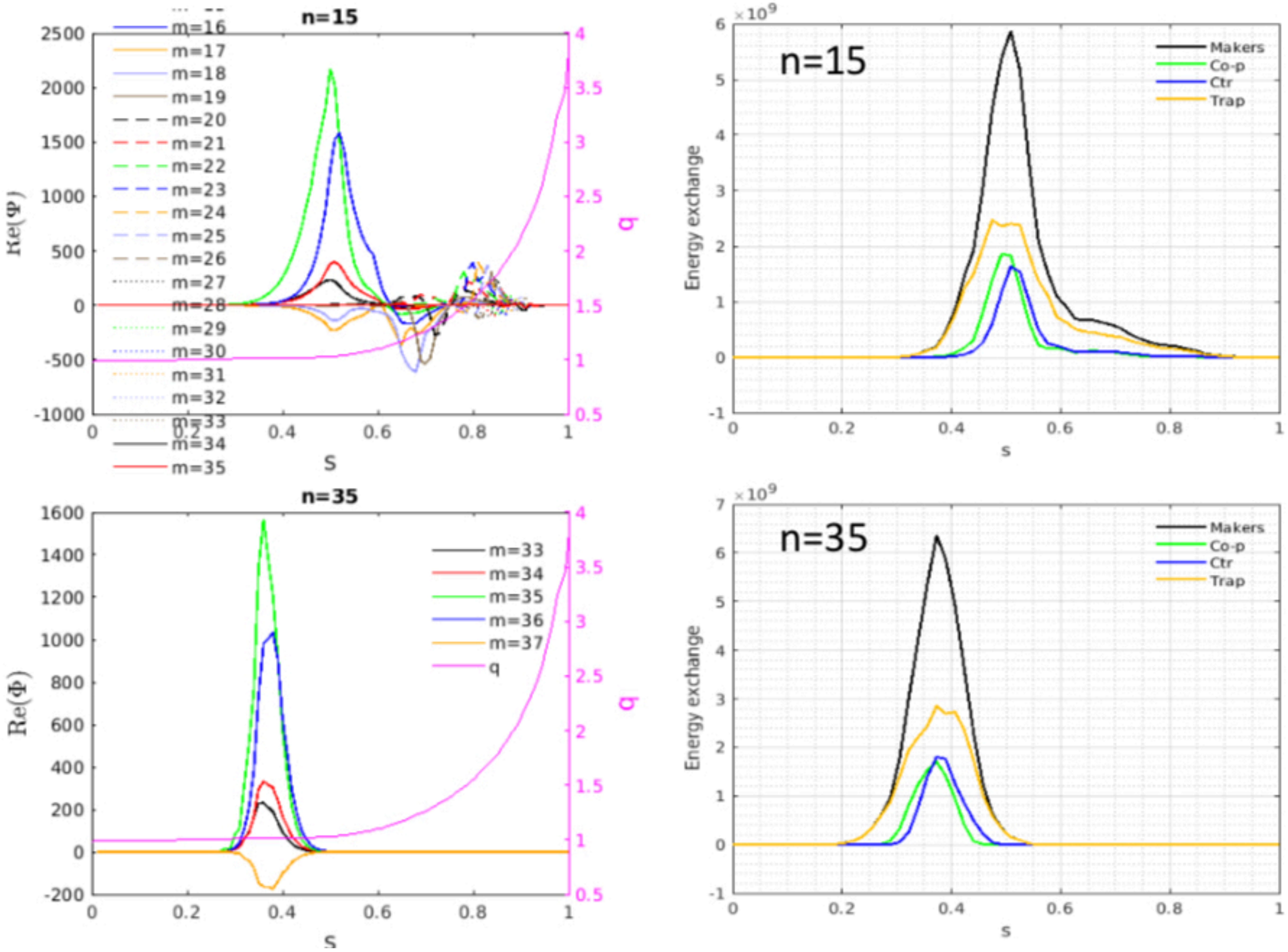
M1: Extend unperturbed orbit integration routines and averaging procedures in order to calculate phase space fluxes in HAGIS

M2: Explore methodology and possibly implement RABBIT as EP source into HAGIS

M3: Finish reduced EP transport workflow based in LIGKA/HAGIS within IMAS

EP fluxes based on EP energy exchange:

- separation wrt particle species (passing/trapped)
- test particle analysis; global/local
- extend to multi-resonance/mode cases
- connection to WP 3.1



M1: in IMAS: appropriate orbit intergral data fields exist already

distribution(i1)/markers(itime)/orbit_integrals

5d: type,marker, n,m,k

Integrals along the markers orbit. These dimensionless expressions are of the form: (1/tau) integral (f(n_tor,m_pol,k,eq,...) dt) from time - tau to time, where tau is the transit/trapping time of the marker and f() a dimensionless function (phase factor,drift,etc) of the equilibrium (e.g. q) and perturbation (Fourier harmonics n_tor,m_pol and bounce harmonic k) along the particles orbits. In fact the integrals are taken during the last orbit of each marker at the time value of the time node below

distribution(i1)/markers(itime)/orbit_integrals_instant

Integrals/quantities along the markers orbit. These dimensionless expressions are of the form: (1/tau) integral (f(eq) dt) from time - tau to time_orbit for different values of time_orbit in the interval from time - tau to time, where tau is the transit/trapping time of the marker and f(eq) a dimensionless function (phase, drift,q,etc) of the equilibrium along the markers orbits. The integrals are taken during the last orbit of each marker at the time value of the time node below

call hagis2(equilibrium_in=equilibrium_ingf,distribution_in= distribution_ingf,distribution_out=distribution_outgf,code_parameters_buffer= buffer_hagis2)

to be done: add perturbations - kick-model equivalent information

IMAS resources: LIGKA/HAGIS/EP-WF

IDS data model: https://sharepoint.iter.org/departments/POP/CM/IMDesign/Data%20Model/CI/imas-3.32.0/html_documentation.html

LIGKA: https://git.iter.org/projects/STAB/repos/ligka/commits

HAGIS: https://git.iter.org/projects/STAB/repos/hagis/browse

EP-WF: https://git.iter.org/projects/WF/repos/ep-stability-wf/browse

short documentation EP WF: https://confluence.iter.org/pages/viewpage.action?pageId=289069024

1 Resources

Some of the resources I found useful when building the Python version of the WF

1. **https://confluence.iter.org/display/IMP/Integrated+Modelling+Home+Page** -> for keeping track of new version of IMAS/PyAL/FC2K (very important!!)
   (a) **https://jira.iter.org/projects/IMAS?selectedItem=com.atlassian.jira.jira-projects plugin:release-pagestatus=released** -> IMAS dictionary changes
   (b) **https://confluence.iter.org/display/IMP/Access+Layer** -> HDF5 or MDS+ back-end for Python
2. **https://user.iter.org/?uid=YSQENWaction=get_document** -> Backend functions documentation for retrieving/manipulating/storing data (Not only Python but also Fortran, C++ and Java)
3. **https://docs.psnc.pl/display/WFMS/FC2K+Python+wrapper+redesign** -> FC2K actor wrapper design (useful for calling an actor after being wrapped by python)
4. **https://confluence.iter.org/display/IMP/iWrap+Python+Actor** -> how to build a pytho actor
5. **https://confluence.iter.org/display/IMP/4.1+FC2K+Basics** -> small FC2K tutorial for kepler, but the same can be used for Python (just select the python generation)
6. **https://confluence.iter.org/display/IMP/3.2+Fortran+examples** -> 4 examples of Fortran code with IDSs
7. **https://confluence.iter.org/display/IMP/iWrap+-+Fortran+API** -> Fortran API (can be used with FC2K to generate an actor that can be used in python wf)
8. **https://confluence.iter.org/pages/viewpage.action?pageId=289069024** -> working example of the EP WF.
9. **Use the first link to keep track of the working versions of each dependency (most of them do not have backward compatibility!!)**

2 Example

In order to be able to connect the numerical tools with IMAS and to be able to perform time-dependent analysis on any scenario, Energetic Particle Stability Workflow was created. This is the first time-dependent workflow which uses IMAS infrastructure to perform Energetic particle analysis. It is written in Python and makes use also of a simple interface which makes parameter configuration easy for both the connection to the IMAS Database (for saving/retrieving data) and for the numerical codes themselves through a series of XML files. A general layout of the components that the workflow uses can be seen in Fig.1.

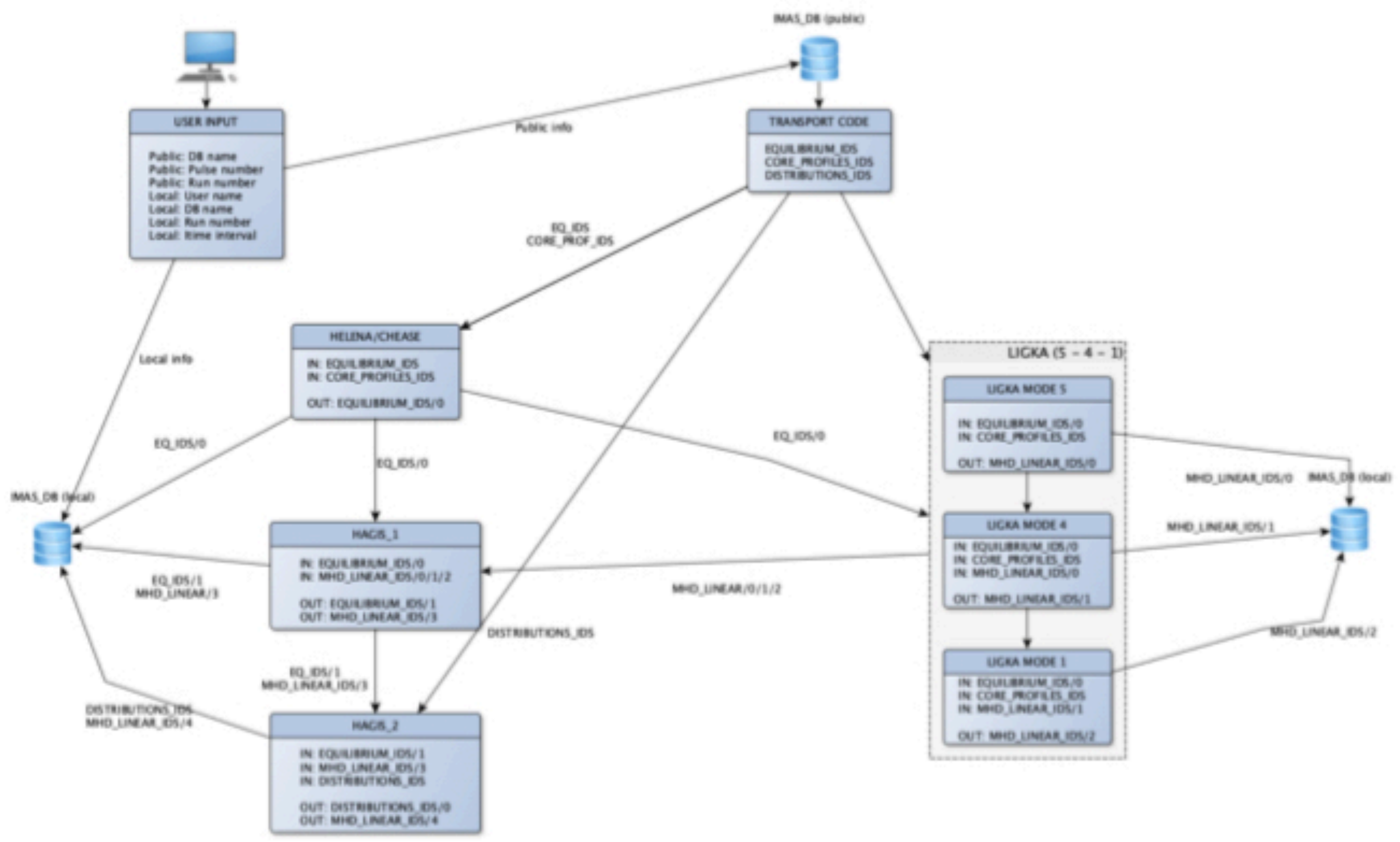


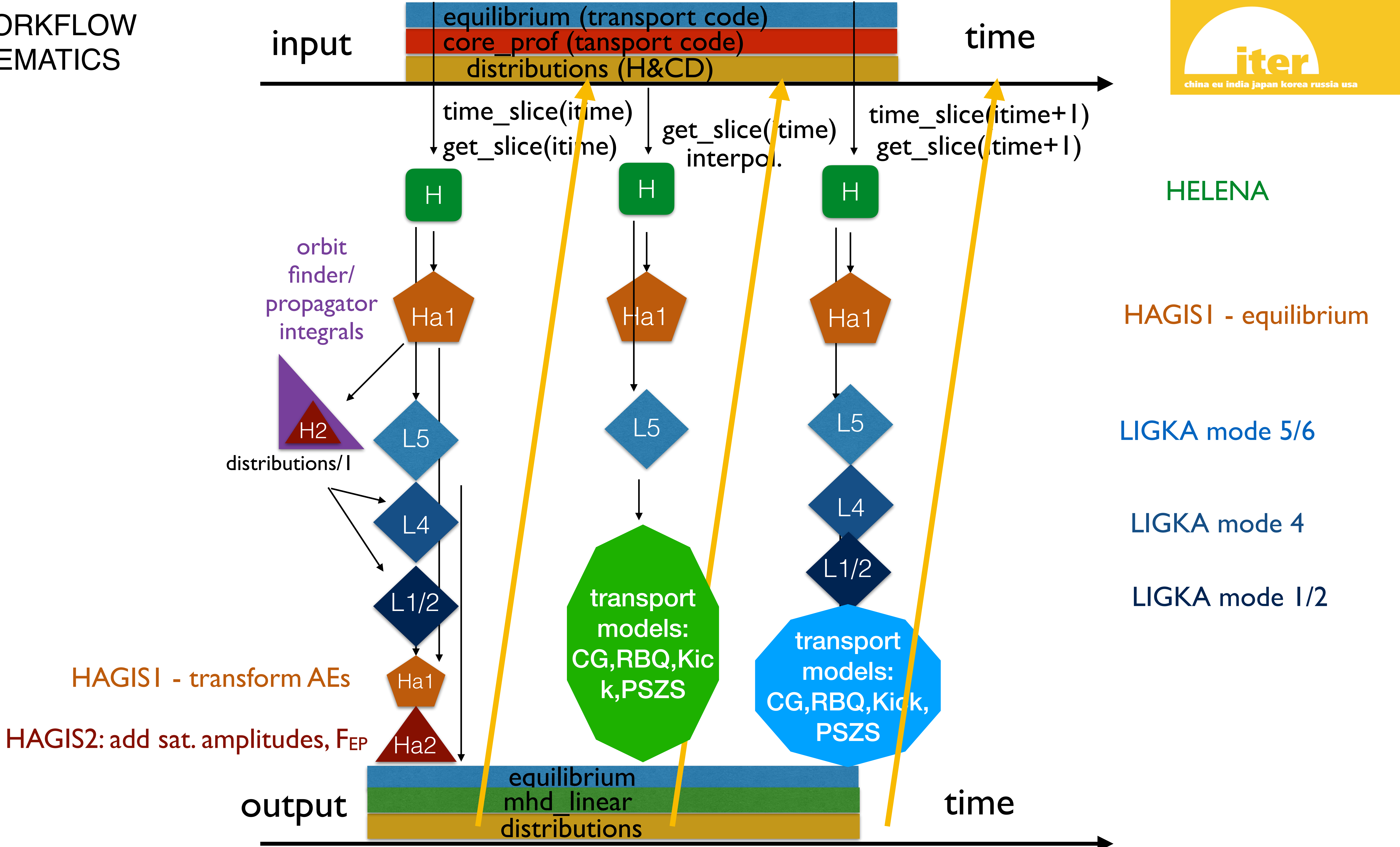
Figure 1: Energetic Particle Stability Workflow general layout of the components.

Now the example that we will use is a MPI actor (mode 4 of LIGKA): Before the actor can be used one needs to import it in python as follows: **from ligka.wrapper import ligka_actor**

Figure 2: Example of a typical actor inside a WF.

An example of a working FC2K is the ligka actor: load modules from EP WF by following the tutorial in the confluence page. Then clone ligka and in root of the dir **fc2k** command. Then open the file named **ligka_WF-PY.xml** and check out the parameters/compare them with the ones in the documentation.

EP WORKFLOW SCHEMATICS



next steps:

- implement explicit expressions needed for PSZS model (probably as HAGIS module?)
- define where shared development of model/implementation is possible
- further collaboration with WP 3.1
- define connection to transport code IDSs

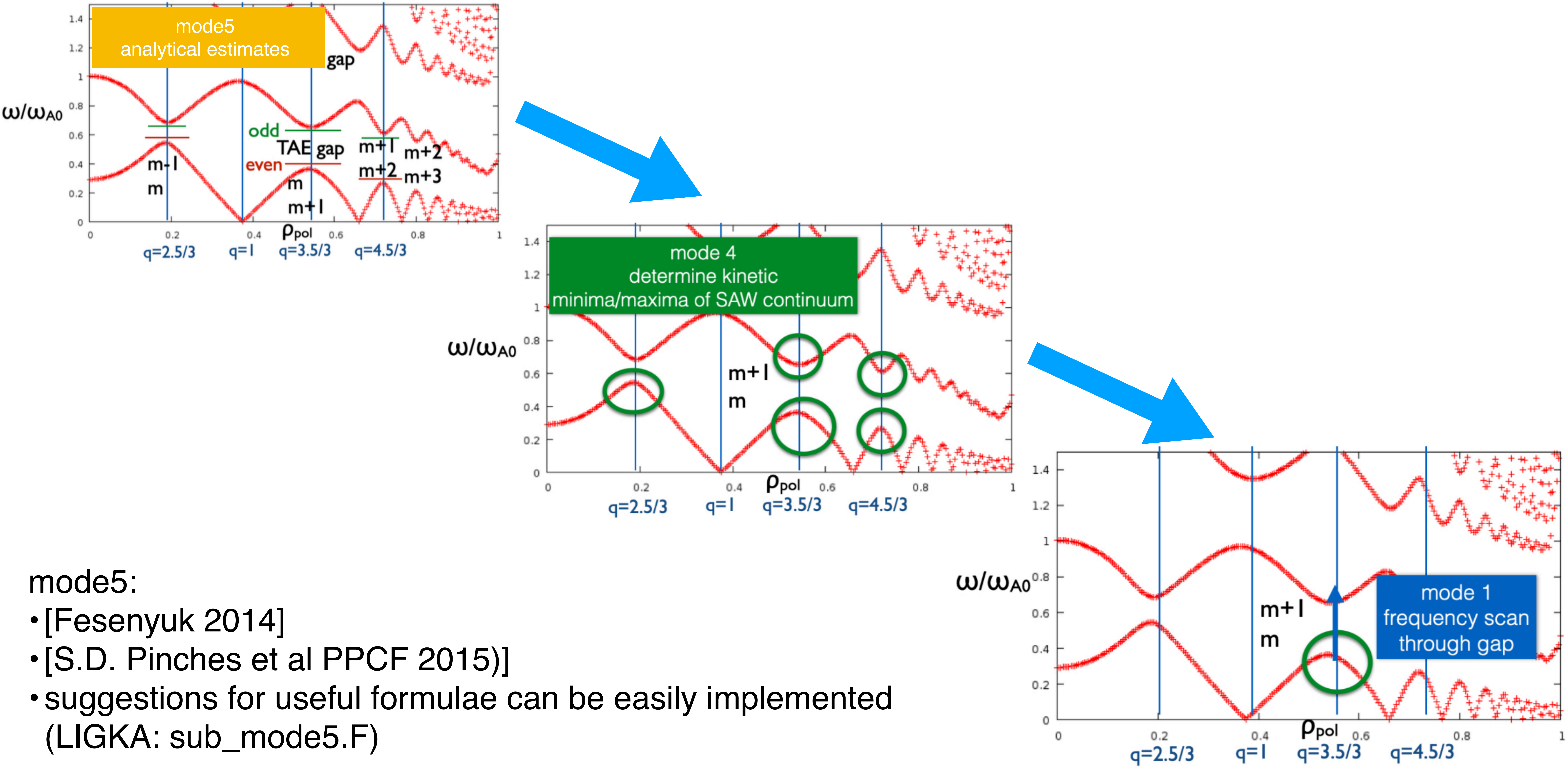
additional slides

discussion and action items

dedicated discussion on DEAPS/LIGKA benchmark/common development
dedicated meeting on IMAS in 1-2 weeks?
dedicated meeting on role of RABBIT?
aligned discussion with TSVV on experimental cases (JET DT)

next general meeting? end of July?

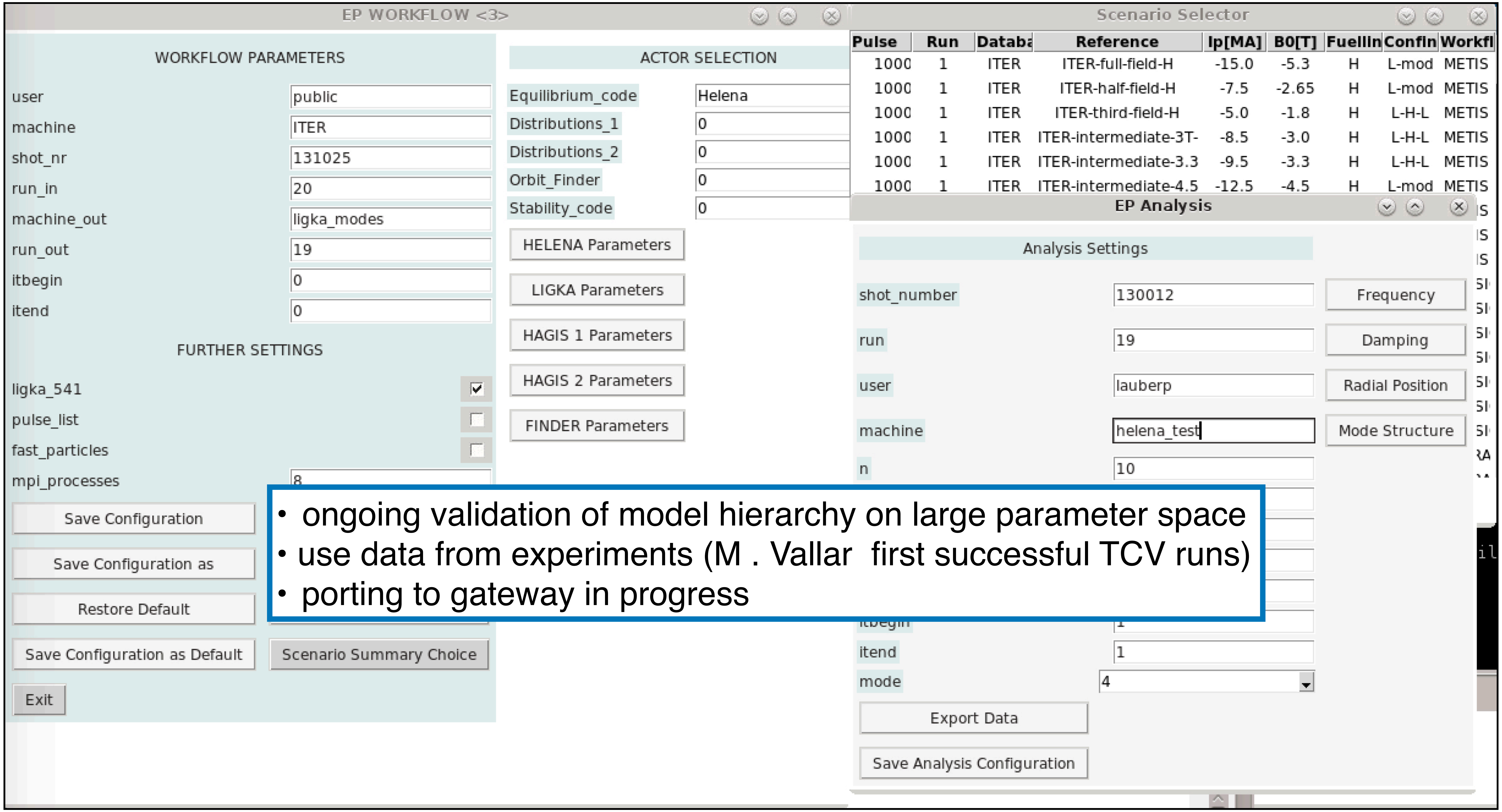
combination of models lead to a staged approach for automated analysis



mode5:

- [Fesenyuk 2014]
- [S.D. Pinches et al PPCF 2015)]
- suggestions for useful formulae can be easily implemented (LIGKA: sub_mode5.F)

interactive, gui, no-gui versions available [V.-A. Popa]



- ongoing validation of model hierarchy on large parameter space
- use data from experiments (M . Vallar first successful TCV runs)
- porting to gateway in progress

linear model equations containing crucial effects for self-consistent description of EP driven modes:

gyrokinetic equation:

unperturbed orbits — propagator → resonance — free energy

$$h = \frac{ie}{T} F_0 \sum_m \int_{-\infty}^{t} dt' e^{i[n(\varphi'-\varphi)-m(\theta'-\theta)-\omega(t'-t)]} e^{-im\theta} \cdot (\omega - \omega_*^T) J_0 \cdot \left[\phi_m(r') - (1 - \frac{\omega_d(\theta')}{\omega})\psi_m(r')\right]$$

quasi-neutrality:

polarisation

$$\sum_a \frac{e_a^2 n_a}{T_a} \left[\varrho_a^2 \nabla_\perp^2\right] \phi + e_a \int J_0 f \; d^3\mathbf{v} = 0; \qquad \mathbf{E} = -\nabla\phi - \frac{\partial \mathbf{A}}{\partial t}; \qquad A_\parallel = \frac{1}{i\omega}(\nabla\psi)_\parallel$$

gyrokinetic moment equation:

shear Alfven law

$$-\frac{\partial}{\partial t}\left[\nabla \cdot (\frac{1}{v_A^2}\nabla_\perp \phi)\right] + (\mathbf{B}\cdot\nabla)\frac{\nabla \times \nabla \times \frac{c}{i\omega}(\nabla\psi)_\parallel}{B^2} + \left[\frac{1}{i\omega}\nabla(\nabla\psi)_\parallel \times \mathbf{b}\right] \cdot \nabla \frac{\mu_0 j_{0\parallel}}{B}$$

$$= -\sum_a \mu_0 \int d^3v (e\mathbf{v}_d \cdot \nabla J_0 f)_a + \frac{3}{4}\frac{\mu_0 e_a^2 n_a}{T_a} \varrho_a^4 \nabla_\perp^4 \frac{\partial}{\partial t}\phi + \sum_a \frac{m_a n_a}{m_i n_i}\frac{\omega_a^*}{v_A^2}\nabla_\perp^2 \phi$$

'pressure' tensor - curvature drift coupling

originally based on H. Qin, PhD Thesis 1998, PoP 1999

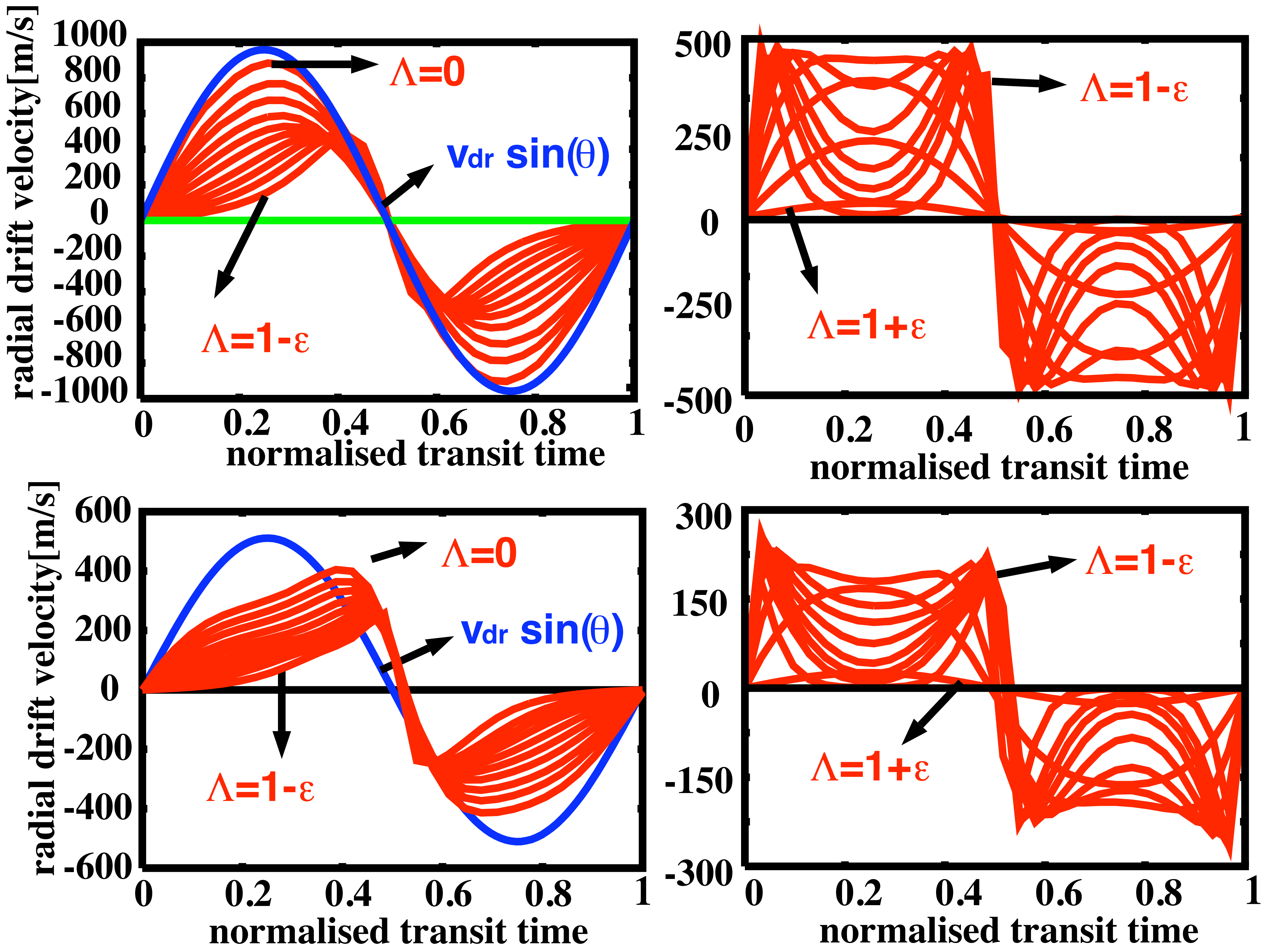
reduced MHD as limit

$E_{//}=0$

coefficients can be calculated using the finder programme, included in LIGKA git repository

geodesic curvature $\omega_d^r = (\mathbf{v}_d \cdot \nabla)_r \approx \sin(\theta) \frac{v_{thi}^2}{\Omega_{ci} R_0} \frac{\partial}{\partial r}$ (circular geometry)

circulating/ centre
κ=1.2



trapped/ centre

circulating/ edge
κ=1.45

trapped/ edge

upgrade analytical expression building on [I. Chavdarovski et al, 2014…]

FOW dispersion relation for LIGKA

$$\omega^2\Big(1-\frac{\omega_{*p}}{\omega}\Big)-k_\parallel^2\omega_A^2R_0^2=2\frac{v_{thi}^2}{R_0^2}\Bigg(-\Big[H(x_{m-1})+H(x_{m+1})\Big]+$$
$$\tau\Big[\frac{N^m(x_{m-1})N^{m-1}(x_{m-1})}{D^{m-1}(x_{m-1})}+\frac{N^m(x_{m+1})N^{m+1}(x_{m+1})}{D^{m+1}(x_{m+1})}\Big]\Bigg)$$

no FOW,
circulating particle
approximation

[Zonca 1996,2009 Lauber 2009]

$$\Big(\frac{N_{-1,0}N^G{}_{0,-1}}{D_{-1,-1}}+\frac{N_{1,0}N^G{}_{0,1}}{D_{1,1}}\Big)+$$
$$\rho^2\Big[D_{0,0}\Big[D_{-2,-2}D_{1,1}D_{-1,-1}\Big(D_{2,2}\Big(D_{-1,-1}\left(Q_{1,0}N^G{}_{0,1}+N_{1,0}Q^G{}_{0,1}\right)-$$
$$F_{-1,1}\left(N_{1,0}N^G{}_{0,-1}+N_{-1,0}N^G{}_{0,1}\right)\Big)$$
$$-D_{-1,-1}\left(E_{1,2}P_{2,0}N^G{}_{0,1}+E_{2,1}N_{1,0}P^G{}_{0,2}\right)\Big)+$$
$$D_{1,1}^2\Big(D_{2,2}\Big(E_{-2,-1}N_{-1,0}\left(E_{-1,-2}N^G{}_{0,-1}-D_{-1,-1}P^G{}_{0,-2}\right)+$$
$$D_{-1,-1}P_{-2,0}\left(D_{-1,-1}P^G{}_{0,-2}-E_{-1,-2}N^G{}_{0,-1}\right)+$$
$$D_{-2,-2}\left(D_{-1,-1}\left(Q_{-1,0}N^G{}_{0,-1}+N_{-1,0}Q^G{}_{0,-1}\right)-F_{-1,-1}N_{-1,0}N^G{}_{0,-1}\right)\Big)+$$
$$D_{-2,-2}D^2_{-1,-1}P_{2,0}P^G{}_{0,2}\Big)+D_{-2,-2}D^2_{-1,-1}N_{1,0}N^G{}_{0,1}\left(E_{1,2}E_{2,1}-D_{2,2}F_{1,1}\right)\Big]$$
$$+D_{-2,-2}D_{2,2}\Big(D_{1,1}\left(E_{0,-1}N_{-1,0}-D_{-1,-1}P_{0,0}\right)+$$
$$D_{-1,-1}E_{0,1}N_{1,0}\Big)\Big(D_{1,1}\left(E_{-1,0}N^G{}_{0,-1}-D_{-1,-1}P^G{}_{0,0}\right)+D_{-1,-1}E_{1,0}N^G{}_{0,1}\Big)\Big]/$$
$$\left(D_{-2,-2}D^2_{-1,-1}D_{0,0}D^2_{1,1}D_{2,2}\right)$$

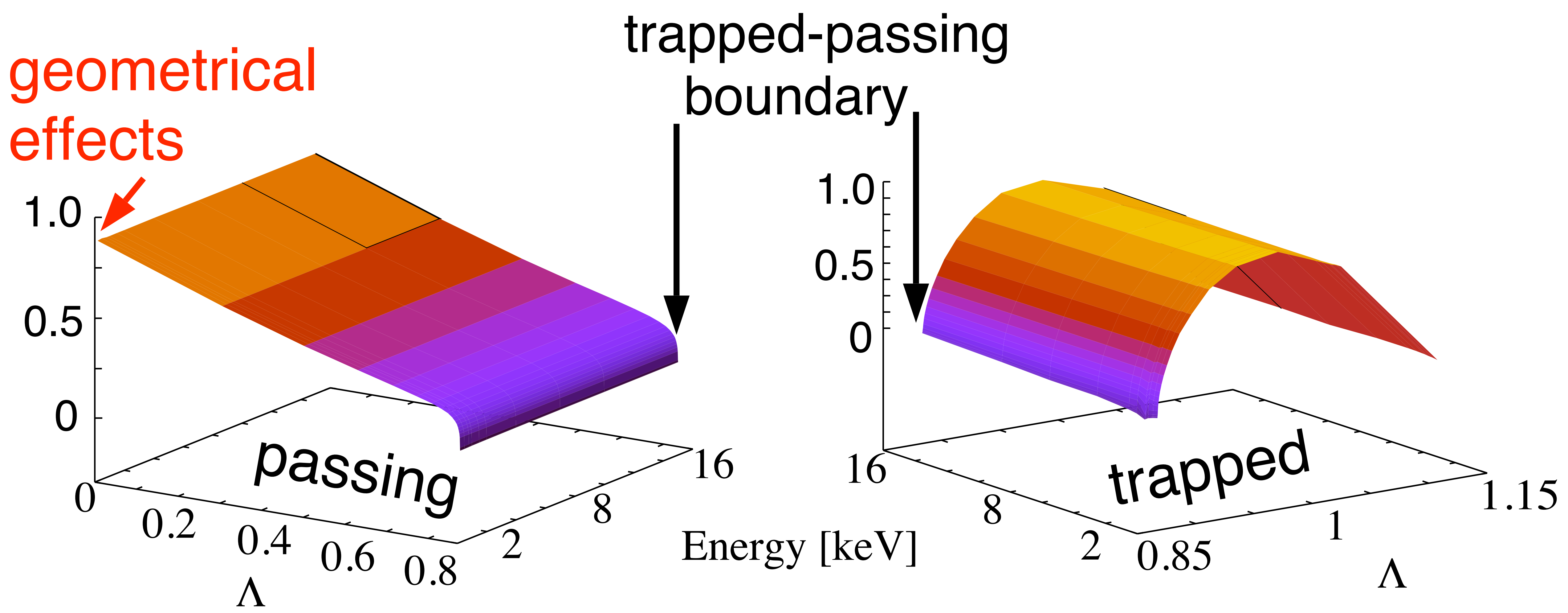
2nd order FOW

[Zonca 1998, Z.X. Lu 2017,Lauber JPC 2018]

- equivalent to EGAM FOW equations: Qiu [2009], Miki & Idomura [2015]
- fast analytical model for FOW effects: solve equations both locally (scan k_r) and globally
- LIGKA mode (3/4 , specification of kr needed)
- rationale: implement global effects in local model - can be improved by estimating analytically AE mode structures (ongoing…)

analytical expression/result:

$$a^G_{k,\sigma} = \frac{1}{\tau_t \omega}\int_0^{\tau_t} dt\left[\omega_d^\theta \cos(\theta) + \frac{\omega_d^r}{i}\sin(\theta) + \omega_{prec}\right]e^{i\sigma k \omega_t t} = \frac{\delta_{k,\pm 1}}{2\omega}(\omega_d^\theta \mp \omega_d^r) + \delta_k \omega_{prec}$$



dependence on pitch angle, substantial deviations for low frequencies

EUROfusion

with

$$\tilde{D}^m(x) = (1 - \frac{\omega_*^m}{\omega}) x Z(x) - \frac{\omega_*^m}{\omega}\eta\Big(x^2 + xZ(x)(x^2 - \frac{1}{2})\Big)$$

$$2\tilde{N}^m(x) = (1 - \frac{\omega_*^m}{\omega})\Big[x^2 + xZ(x)(x^2 + \frac{1}{2})\Big] - \frac{\omega_*^m}{\omega}\eta\Big[x^2(x^2 + \frac{1}{2}) + xZ(x)(\frac{1}{4} + x^4)\Big]$$

$$P = \tau(\Gamma_0 - 1)\Big[1 - \frac{\omega_i^*}{\omega}\Big(1 + \eta_i \frac{\Gamma_0 G_0}{\Gamma_0 - 1}\Big)\Big].$$

$$H^m(x_m) = \tilde{H}^m(x_{m,i}) + \tau \tilde{H}^m(x_{m,e}) \text{ and } \tilde{H}^m(x) = \frac{1}{2}\Big[(1 - \frac{\omega_*^m}{\omega})\tilde{F}(x) - \eta\frac{\omega_*^m}{\omega}\tilde{G}(x)\Big],$$

$$2\tilde{F}(x) = xZ(x)(\tfrac{1}{2} + x^2 + x^4) + \frac{3x^2}{2} + x^4,$$

$$2\tilde{G}(x) = xZ(x)(\tfrac{3}{4} + x^2 + \tfrac{x^4}{2} + x^6) + 2x^2 + x^4 + x^6$$

$$\omega_d^{\pm} \approx \frac{v_{th,i}^2}{\Omega_i}\frac{1}{R_0}(\frac{m}{r} \pm \frac{\partial}{\partial r}) = \omega_d^n \pm \omega_d^r$$

Assuming a Maxwellian F_0 with $\partial F_0/\partial E = -F_0/T$ and using

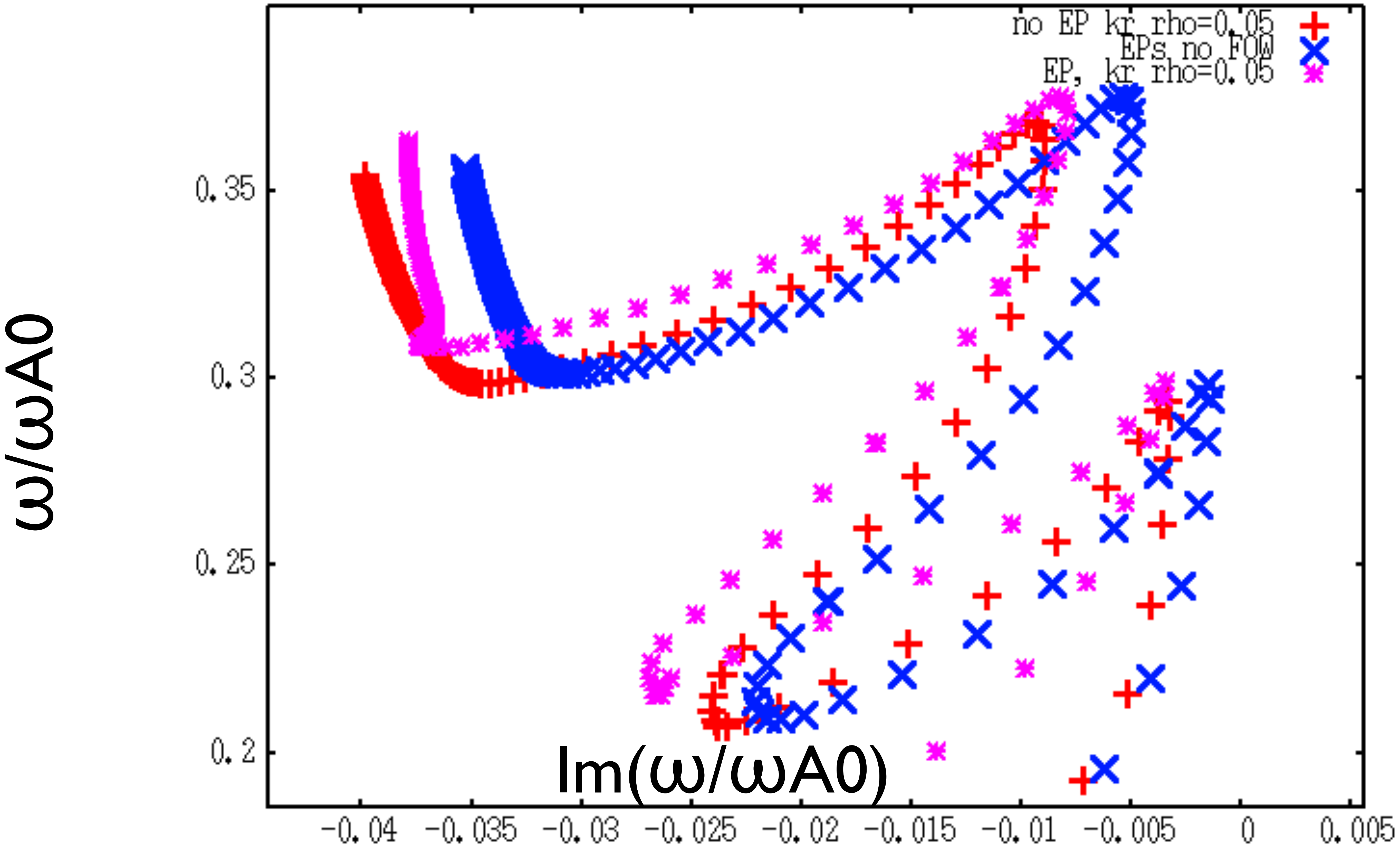
$$\int_0^\infty \frac{dt\ e^{-t^2}}{x_m^2 - t^2} = \frac{-\sqrt{\pi}Z(x_m)}{2x_m}; \qquad \int_0^\infty \frac{dt\ t^2\ e^{-t^2}}{x_m^2 - t^2} = \frac{-\sqrt{\pi}}{2}(x_m + x_m^2 Z(x_m))$$

where

$$x_m = \frac{\omega}{|k_{\parallel,m}| v_{th}}; \qquad t = \frac{v_\parallel}{v_{th}}; \qquad v_{th} = \sqrt{\frac{2T}{m}}$$

$\tau = Te/Ti$

adding Maxwellian αs, T_α=1MeV, $v_{th,\alpha}/v_{A0}$=1.0
$kr \cdot \rho i \sim 0.05$; $kr \cdot \rho_\alpha \sim 0.3$



reduced EP drive in TAE range - as expected, but BAE is stabilised?
2nd order expansion should be valid till $kr \cdot \rho_\alpha \sim 1$
difficult system, since local and global effects are both present via kr