Linear and non-linear benchmark between HYMAGYC, MEGA and ORB5 codes using the NLED-AUG test case to study Alfvénic modes driven by energetic particles

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Outline

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- Setting up of the benchmark
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- Linear benchmark:
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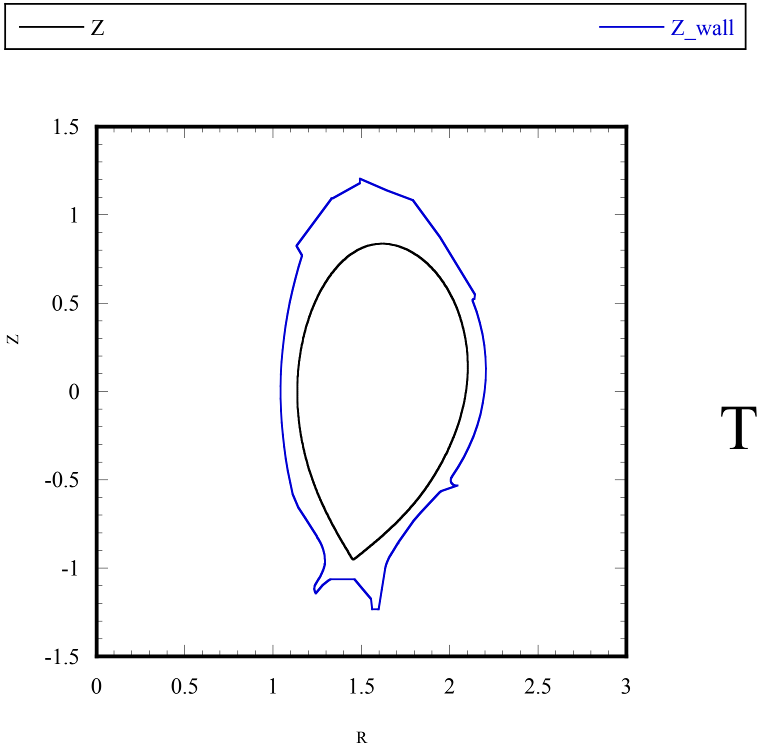
  - Parameter scans: EP density n_H and EP temperature T_H
- Non-linear benchmark
  - Nominal case for peaked off-axis EP density profile
- Conclusions

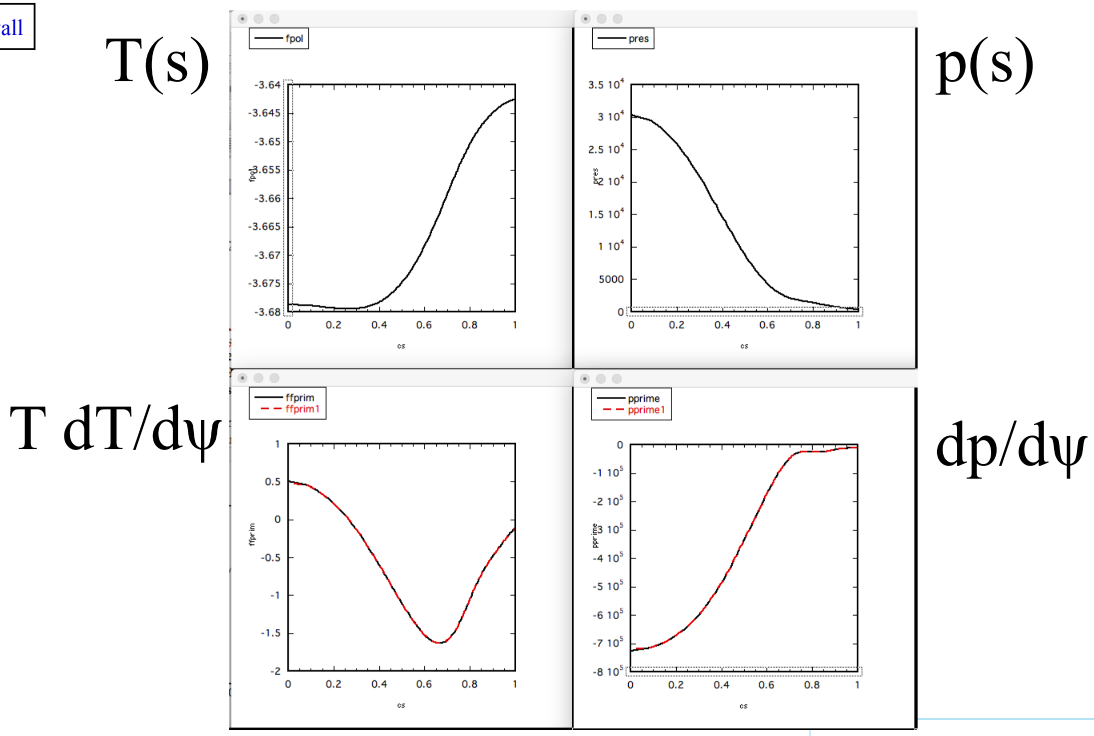
Introduction

- In the frame of the EUROfusion Enabling Research projects MET (*Multi-scale Energetic particle Transport in fusion devices*)[1a] and ATEP (*Advanced Energetic particle transport models*) [1b], a detailed benchmark activity has been undertaken among few of the state-of-the-art codes available to study the self-consistent interaction of an EP population with the shear Alfvén waves, in real magnetic equilibria and in regimes of interest for the forthcoming generation devices (e.g., ITER [2], JT-60SA [3], DTT [4]).
- The codes considered in this exercise are HYMAGYC [5], MEGA [6], and ORB5 [7, 8], the first two being hybrid MHD-Gyrokinetic codes (the bulk plasma is represented by MHD equations, while the EP species is treated using the gyrokinetic formalism), the third being a global electromagnetic gyrokinetic code (both bulk and EP species are treated using the gyrokinetic formalism).
- Similar benchmarks have been done in the past (also within the ITPA EP Topical Group, see, e.g., *Koenies et al., Nuclear Fusion, 58:126027, 2018*): here we decided to use a realistic, shaped cross section, equilibrium from AUG proposed by Philipp Lauber.

Equilibrium

- AUG test case proposed by Philipp Lauber
- Shot considered is AUG #31213, at t=0.84s (shortly, #31213@0.84s), see http://www2.ipp.mpg.de/~pwl/NLED_AUG/data.html
- In order to use such test case to benchmark HYMAGYC on a realistic, fully shaped equilibrium, we have considered the experimental EQDSK g031213.00003





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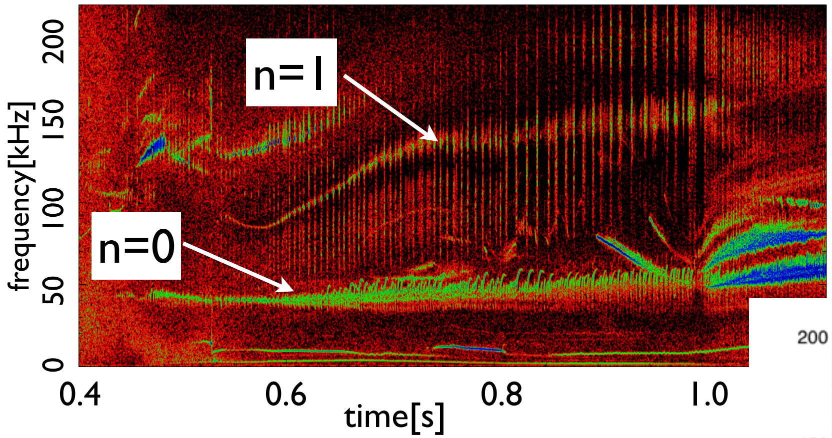
AUG experimental reference case #31213

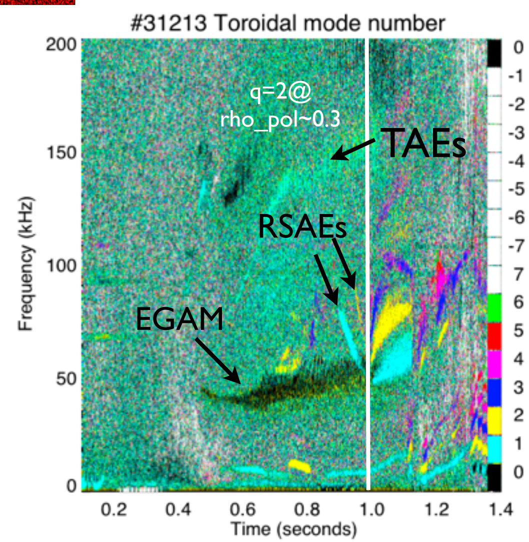
From Ph. Lauber notes, NLED_AUG_benchmark_case.pdf:

ASDEX Upgrade: early off-axis NBI drive [93keV]: bursting EGAMs, RSAEs and TAE/EPMs



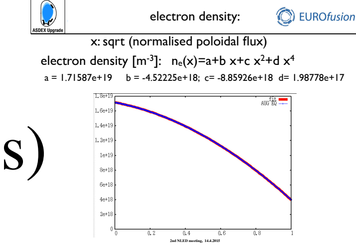
[July 2014]

B0=2.2T
I=0.6-1.0MA
P_{beam}=2.5MW

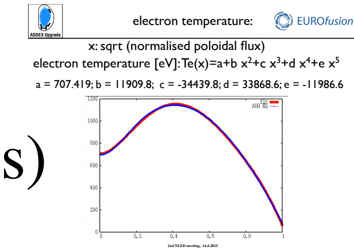


- rather well reproducible scenario
- no 'sea' of Alfvenic modes (TAEs/RSAEs)
- but strongly chirping n=0 modes and n=1 'bursts'

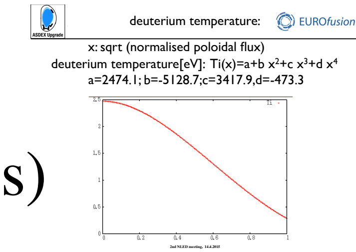
$n_e(s)$



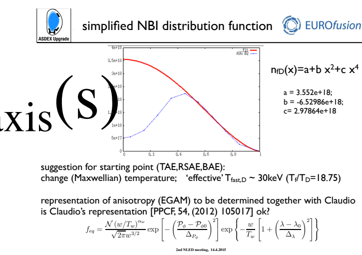
$T_e(s)$



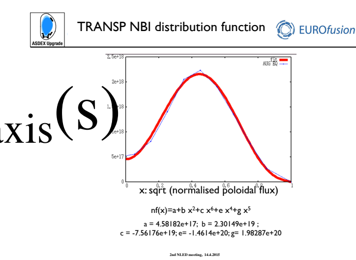
$T_i(s)$



$n_{H,on-axis}(s)$



$n_{H,off-axis}(s)$



2nd NLED meeting, 14.4.2015

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Setting up of the benchmark equilibrium and parameters

The so-called NLED-AUG [9] reference case has been considered, both for the peaked off-axis and peaked on-axis EP density profile cases, using its shaped cross section version. This case poses an exceptional challenge to the codes due to its high EP pressure, the rich spectrum of experimentally observed instabilities and their non-linear interaction [10].

Particular care has been devoted to consider plasma and numerical parameters as close as possible among the three codes:

- the same input equilibrium file (EQDSK) has been considered;
- ion density profile has been obtained by imposing quasi-neutrality ($Z_i n_i + Z_H n_H = n_e$), as required by ORB5 (here n_i, n_e, n_H are the bulk ions, electrons, and EP densities, respectively (both bulk ion and EPs are assumed to be Deuterons), and Z_i, Z_H their electric charge numbers);
- finite resistivity η and the adiabatic index, $\Gamma = 5/3$, have been assumed for both the hybrid codes (this is the usual choice used in MEGA, where also some viscosity is considered to help numerical convergence; note that HYMAGYC do not include viscosity).
- Only finite orbit width (FOW) effects has been retained for the linear benchmark, and an isotropic Maxwellian EP distribution function of Deuterons with T_H =93 keV, constant in radius, has been considered. Finite Larmor radius (FLR) effects also retained in some cases.

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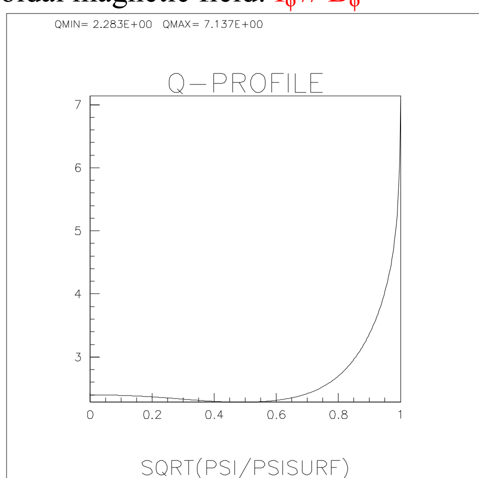
Equilibrium reconstruction

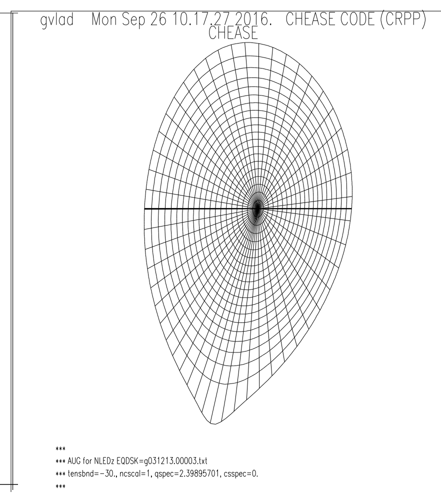
From https://www.afs.enea.it/vlad/Miscellaneous/Benchmark_AUG_testcase_MEGA_ORB5_HYMAGYC_2019/

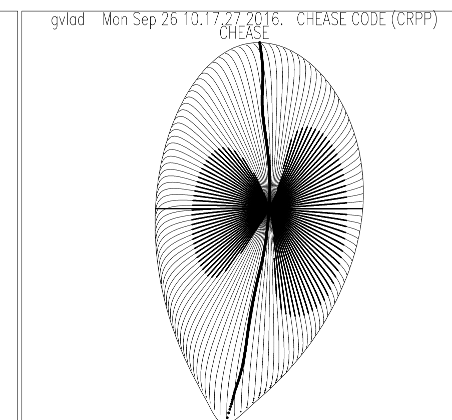
- The file EQDSK g031213.00003 has been used to reconstruct the experimental equilibrium with CHEASE:
  - magnetic field normalization B_0, and length R_0 used in g031213.00003: $B_0=B_{magnetic\text{-}axis}$= -0.220811798E+01, $R_0=R_{magnetic\text{-}axis}$=0.166599977E+0
  - some parameters used in CHEASE:
    - NTMF0=1
    - assign q(s=0) to on-axis q value found in g031213.00003: required to have an "open" toroidal gap: NCSCAL=1, QSPEC=2.39895701, CSSPEC=0.
    - add some smoothing to the boundary to make CHEASE converge more easily: TENSBND=-30.
  - in HYMAGYC (and MARS) use Jacobian: $J \sim R/|\nabla\psi|$
  - Consider an equivalent equilibrium with $B_0 \Rightarrow |B_{magnetic\text{-}axis}|$ and the toroidal current parallel to the toroidal magnetic field: I_ϕ // B_ϕ

Quantity	Value (peaked on-axis case)	Value (peaked off-axis case)	Data definition/Origin
B_mag [T]	2.20811798	2.20811798	EQDSK, magnetic field on the magnetic axis (R=R_mag)
R_mag [m]	1.66599977	1.66599977	EQDSK, magnetic axis major radius
B0 [T]	B0=B_mag	B0=B_mag	normalization coefficient for the magnetic field
R0 [m]	R0=R_mag	R0=R_mag	normalization coefficient for the lengths
R_geo [m]	1.62	1.62	geometric major radius (R_LCMS_max+R_LCMS_min)/2
a [m]	0.48262	0.48262	minor radius (R_LCMS_max-R_LCMS_min)/2
epsilon_dev [m]	0.297898	0.297898	inverse Aspect ratio (a/R_geo)
n_e0 (n_e(s=0)) [10^20/m^3]	0.171587	0.171587	p.17 NLED_AUG_benchmark_case.pdf
n_EP0 (n_EP(s=0)) [10^20/m^3]	0.03552	0.00458182	p.21/p.20 NLED_AUG_benchmark_case.pdf
n_i0 (n_i(s=0)) [10^20/m^3]	0.136067	0.16700518	from n_i(s=0)=n_e(s=0)-n_H(s=0)
n_EP0/n_i0	0.261048	0.0274352	EP density/bulk ion density
m_i/Z_i	2/1	2/1	bulk ion mass/charge (D) (in units of proton mass/electron charge)
m_EP/Z_EP	2/1	2/1	EP mass/charge (D) (in units of proton mass/electron charge)
m_EP/m_i	1	1	mass ratio (EP/bulk ion)
T_EP0 [MeV]	0.093	0.093	on-axis EP Temperature (constant on radius), Maxwellian distribution
v_A0 [m/s]	9.22757x10^6	8.32911x10^6	on-axis Alfvén velocity => 2.18x10^6 B_axis[T]/sqrt(m_i n_i0[10^20/m^3])
tau_A0 [s]	1.80546x10^-7	2.00021x10^-7	R0/v_A0
omega_A0 [rad/s]	5.53876x10^6	4.99947x10^6	1/tau_A0
v_EPth0 [m/s]	2.1111x10^6	2.1111x10^6	sqrt(T_EP0/m_EP) => 9.79x10^6 sqrt(T_EP0[MeV]/m_EP) note the definition w/o sqrt(2)!
v_EPth0/v_A0	0.228782	0.253461	
omega_ci [rad/s]	1.057688x10^8	1.057688x10^8	EP gyrofrequency => 9.58x10^7 Z_EP B0[T]/m_EP
rho_EP0 [m]	0.0199221	0.0199221	on-axis EP Larmor radius (v_EPth0/omega_ci) => 0.102 sqrt(m_EP T_EP0[MeV])/Z_EP/B0[T]
rho_EP0/R0	0.011958	0.011958	on-axis EP Larmor radius/R0
rho_EP0/a	0.041279	0.041279	on-axis EP Larmor radius/a

Table 1.







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Codes and constrains

- MEGA: Hybrid MHD-Gyrokinetic (bulk: nonlinear MHD, Energetic Particles: GK, coupling term: EP current density j'_H) [Todo, Y. & Sato, T. Linear and nonlinear particle-magnetohydrodynamic simulations of the toroidal Alfvén eigenmode. Phys. Plasmas 5, 1321–1327 (1998); Todo, Y., Shinohara, K., Takechi, M. & Ishikawa, M. Computer simulation of frequency sweeping of energetic particle mode in a JT-60U experiment. J. Plasma Fusion Res. 79, 1107–1108 (2003)]

  Main features: (R, Z) coord. (flux coord. for analysis), resistivity η, viscosity ν, adiabatic index Γ in the MHD solver
- ORB5: Fully Gyrokinetic, electromagnetic (bulk (e, i) & Energetic Particles: GK) [E. Lanti et al., Computer Physics Communications (2019)]
- HYMAGYC: Hybrid MHD-Gyrokinetic (bulk: linear, resistive, full MHD, Energetic Particles: GK, coupling term: divergence of EP pressure tensor)) [G. Fogaccia, G. Vlad, S. Briguglio, Nucl. Fusion 56 (2016) 112004]

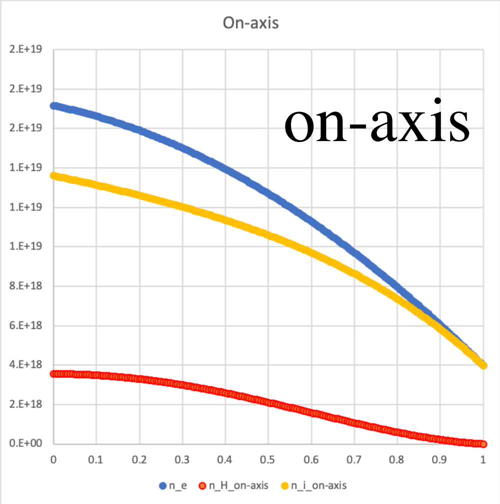
  Main features: (s, χ, ϕ) flux coord., generalized curvilinear coord., can include, in the MHD solver:

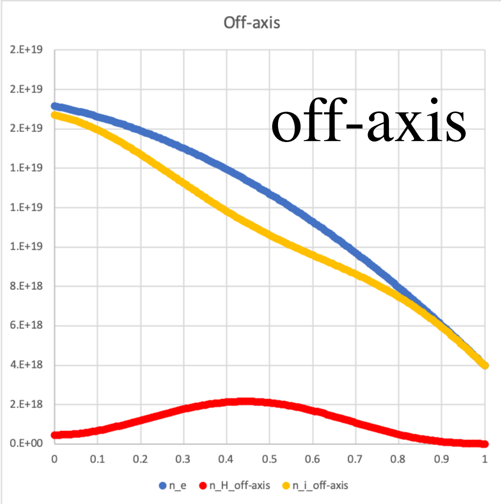
  resistivity η, adiabatic index Γ, (but no viscosity)

Parameters required by each code:

- MEGA: norm. resistivity $S^{-1}_{MEGA}=5\times10^{-7}$ [MEGA units: $S_{MEGA}=\mu_0 R_0 v_{A0}/\eta$, $S_{HYMAGYC}=\mu_0 (a^2/R_0) v_{A0}/\eta$] (HYMAGYC-MEGA)
- MEGA: norm. viscosity $\nu_{norm}=\nu/(R_0 v_{A0})=5\times10^{-7}$
- MEGA: adiabatic index $\Gamma=5/3$ (HYMAGYC-MEGA)
- ORB5: quasi-neutrality $Z_i n_i(s)=n_e(s)-Z_H n_H(s)$ (ORB5-HYMAGYC-MEGA)
- Maxwellian EPs, TH=0.093MeV (ORB5-HYMAGYC-MEGA)

$n_e(s)$, $n_H(s)$ => $n_i(s)$





Characterization of Alfvénic spectra ($|\varphi(s,\omega)|$) in MHD limit

A "decay simulation" experiment, for $n_H=0$ (but now $\Gamma=5/3$, $S^{-1}_{MEGA}=5\times10^{-7}$):

- Toroidal mode number n=1, no EP drive
- MEGA (left) and HYMAGYC (center), ORB5(right) show similar spectra (MEGA exhibits a larger damping)
- two weakly stable TAE modes with lowest damping m=2, 3; ω≈±200 kHz;
- a rich spectrum of global modes;
- SAW Alfvén continua also observed (Falcon code (Falessi et al.) for SAW and ISW continua, log color scale...).

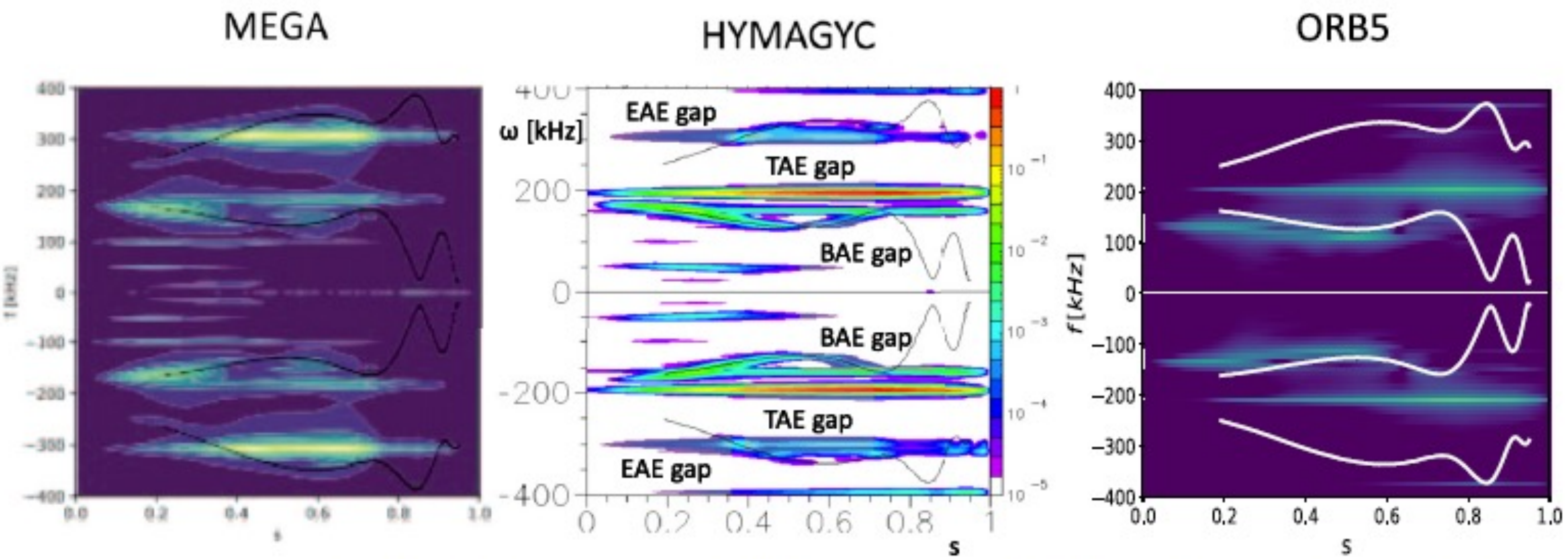


Figure 6. Frequency spectra in the MHD limit for MEGA (left), HYMAGYC (centre), and ORB5 (right). Logarithmic color scale is used for the intensity of the e.s. field $|\varphi(s,\omega)|^2$. Shear Alfvén continuous spectra are also shown using black continuous lines for the MEGA and HYMAGYC spectra, and as white continuous lines for the ORB5 spectra, as obtained by the FALCON code. In the central frame the main gaps are also indicated for reference.

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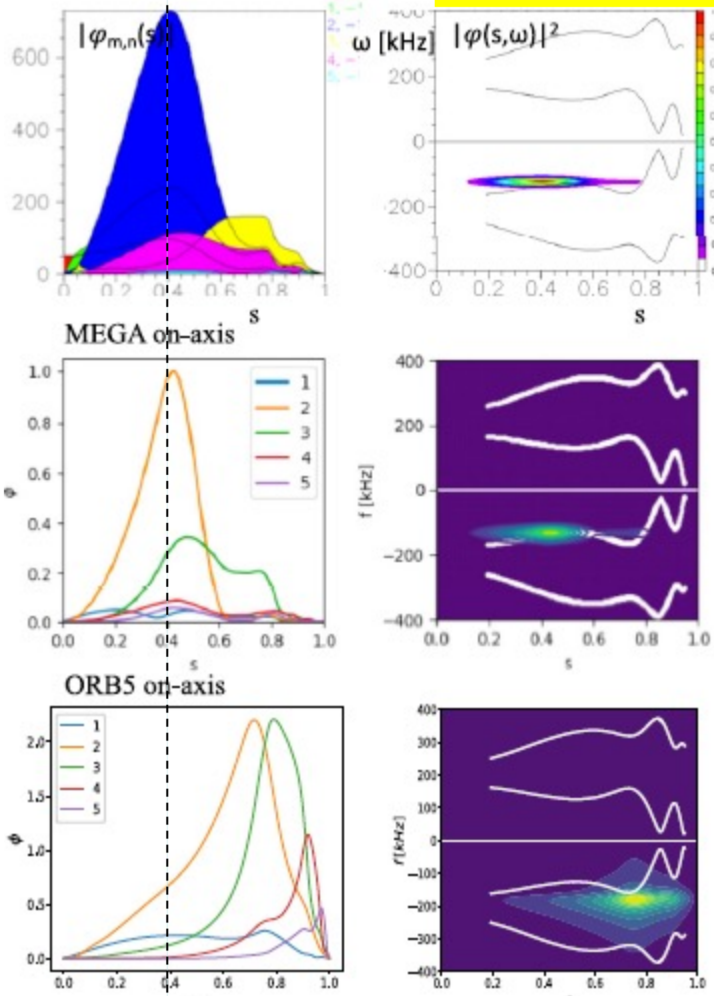
Nominal cases comparison

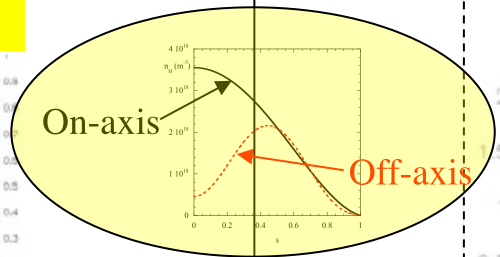
On-axis EPs density profile

$n_{H0}/n_{i0} \simeq 0.261$, $T_H = 0.093$ keV

ω vs. s [kHz]



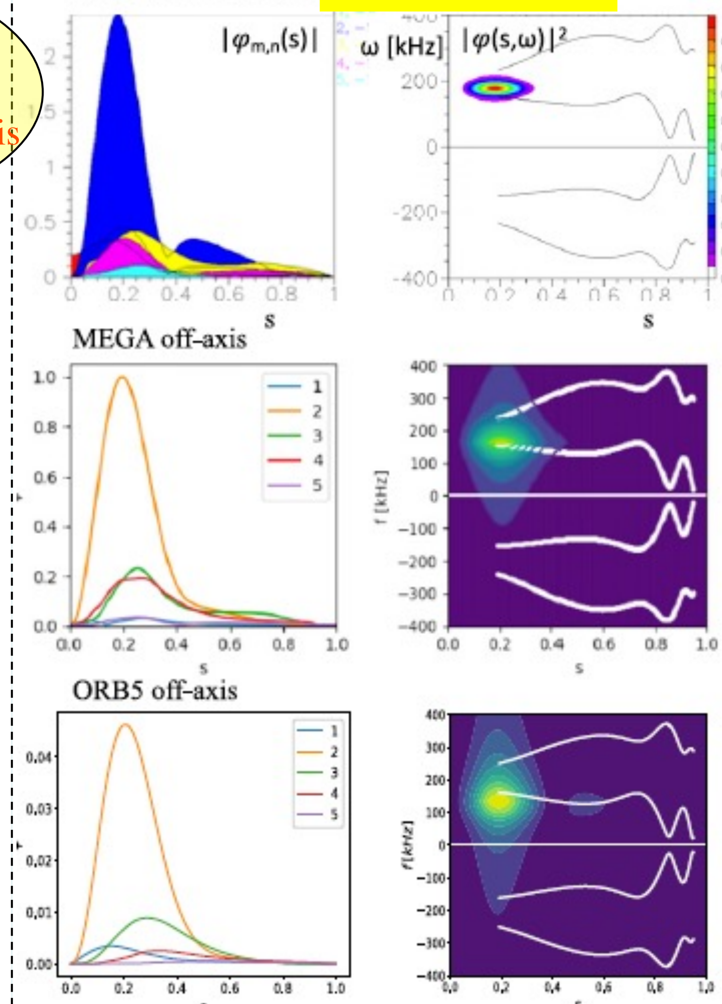
ORB5 mode is similar to TAE in HYMAGYC n_H=0 "decay experiment"



Off-axis EPs density profile

$n_{H0}/n_{i0} \simeq 0.0274$, $T_H = 0.093$ keV

ω vs. s [kHz]



Wave-particle power exchange

- Pattern for the wave-particle power exchange for the on-axis, nominal value, case (HYMAGYC & MEGA) looks very similar (U: normalized Energetic particle parallel velocity, M: normalized Energetic Particle magnetic moment)
- dashed lines correspond to approx. boundary between trapped and circulating particles, for s corresponding to the maximum of the linear eigenfunction location (s ≈ 0.4)

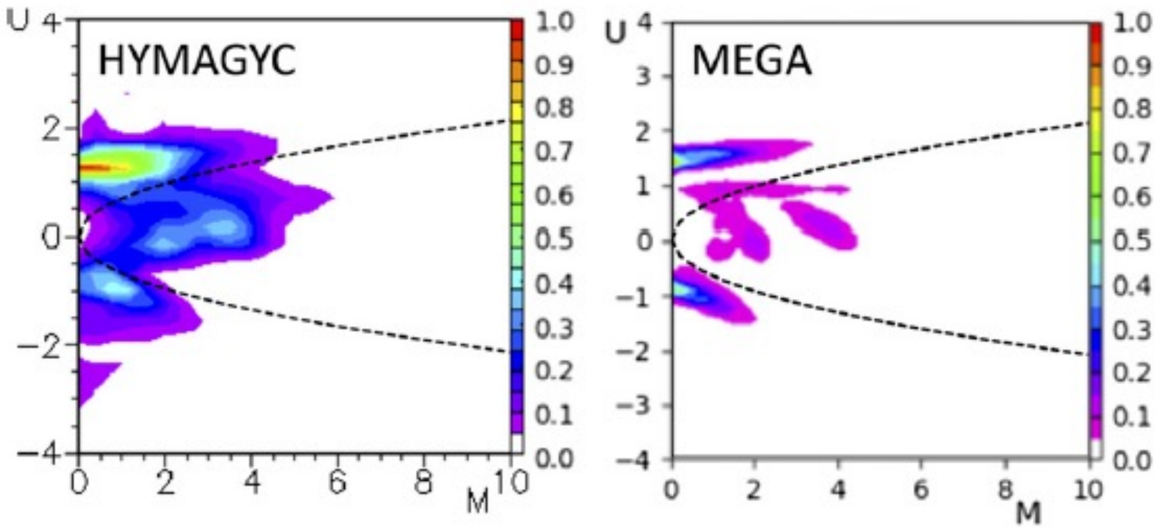
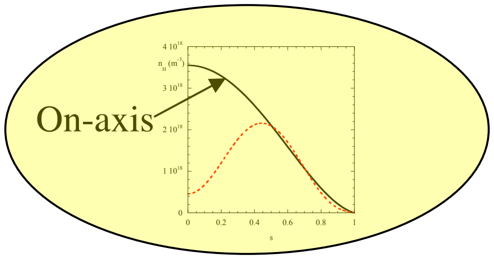


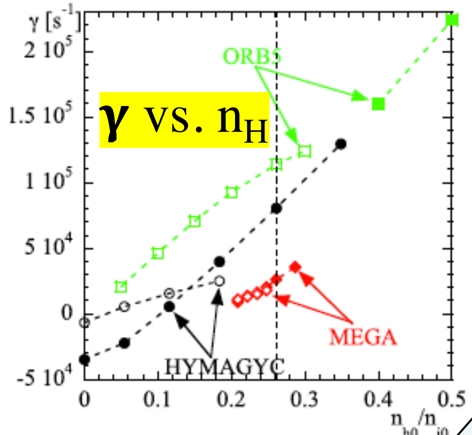
Figure 9. Wave-particle power exchange in the plane $[U, M]$ for the nominal case parameter, peaked on-axis EP density profile. Here U is the normalized (to the EP thermal velocity) EP parallel velocity, and M is the normalized (to T_h/Ω_{h0}, with Ω_{h0} the on-axis EP cyclotron frequency) EP magnetic moment. HYMAGYC result is shown on the left, and MEGA result on the right; red pattern indicates maximum power exchange from EPs to the wave. Also the approximate boundary between trapped and circulating particles (co-passing for positive U values, counter-passing for negative U ones) is drawn, corresponding to the radial region where the mode is maximum ($s \approx 0.4$).

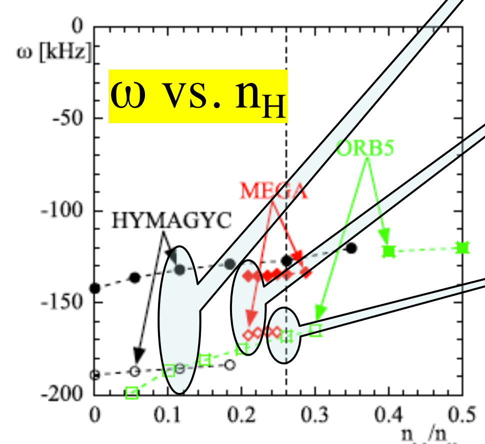
Parameter scans to resolve discrepancy among HYMAGYC, MEGA vs. ORB5 for on-axis EP density profile

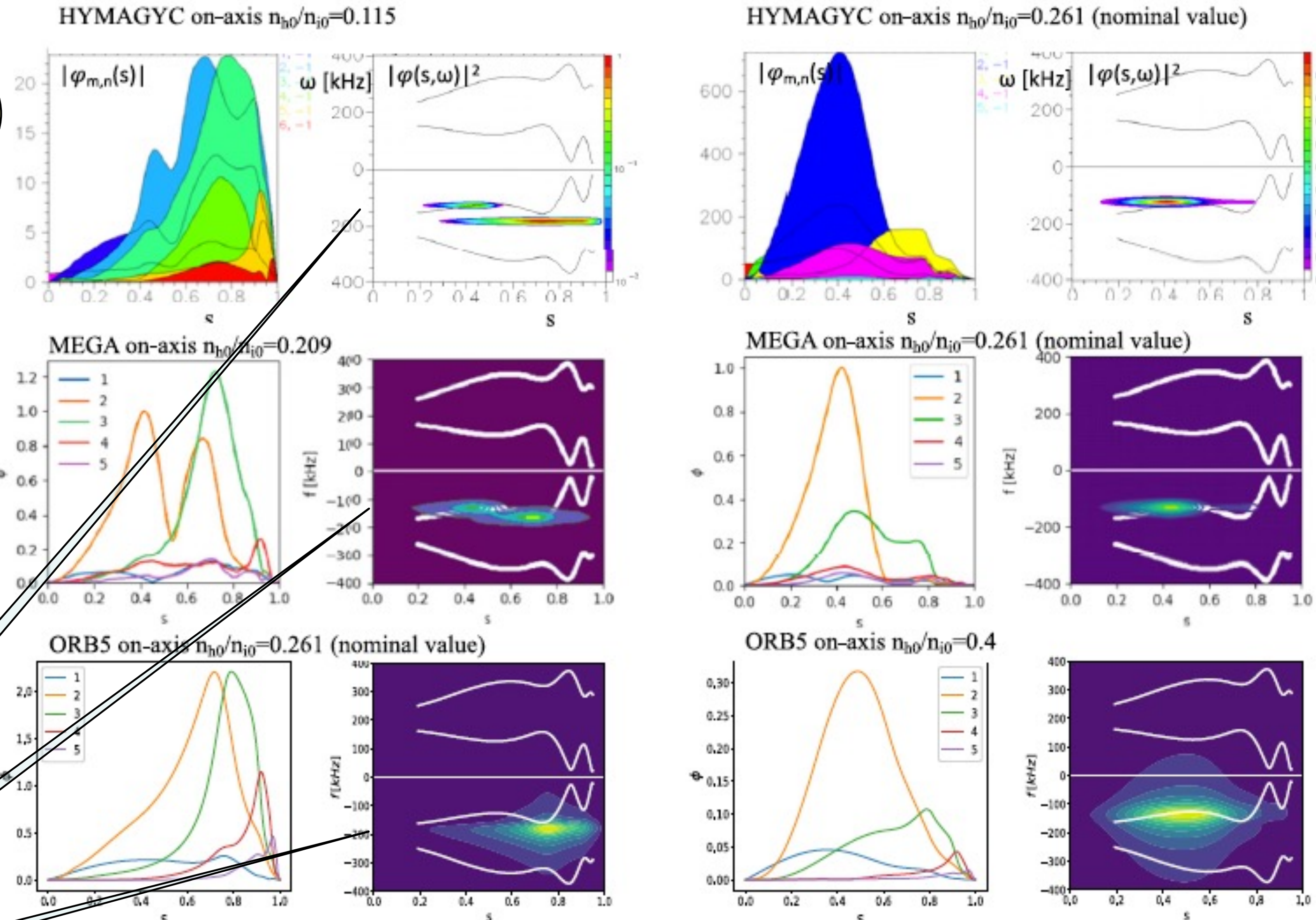
- For the EP density profile peaked on-axis case, ORB5 observes, as the most unstable mode, a TAE located toward the external region of the plasma discharge, whereas HYMAGYC and MEGA observe s more internal mode (RSAE, Reversed shear Alfvén Eigenmode)
- Parameter scans (EP density or EP temperature) allow to reconcile the results of the three codes, showing that all the three codes observes, as the most unstable mode a TAE or a RSAE, depending on the EP density and/or temperature considered
- The occurrence of the 'cross-over' between RSAE and TAE depends strongly on the different damping experienced by the codes, which reflects in considerable variations of the net growth rates observed for this particular case (peaked on-axis EP density profile).
- Nevertheless, when looking carefully to the dependence of the growth rates on the EP density and temperature, all the three codes show quite similar slopes, reflecting a similar EP drive.
- It is to be noted that in this benchmark we are comparing the net growth rate obtained by the three codes, while, e.g., in other benchmark exercises, only the EP drive was compared (*Koenies et al., Nuclear Fusion, 58:126027, 2018*)

Energetic particle n_H scan for on-axis EP density profile-1









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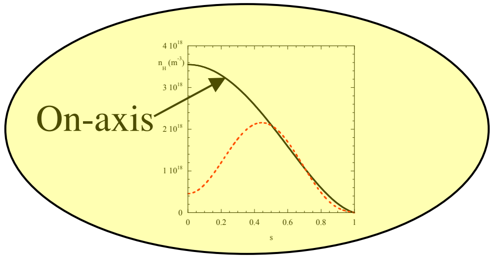
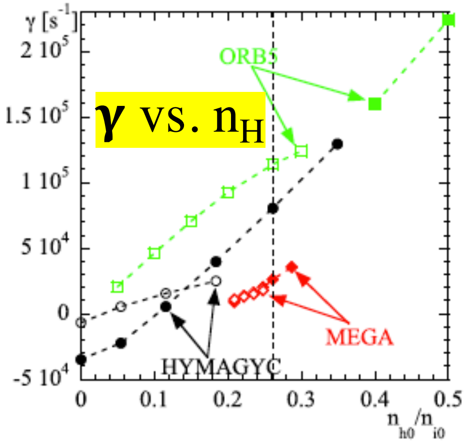
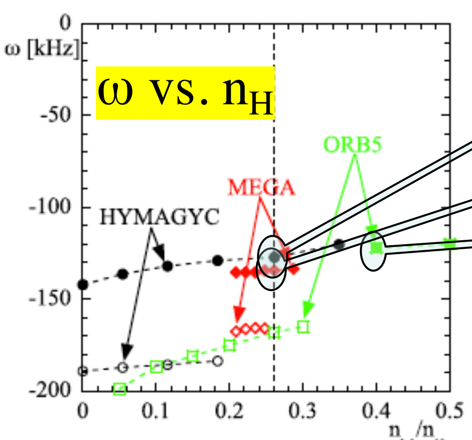
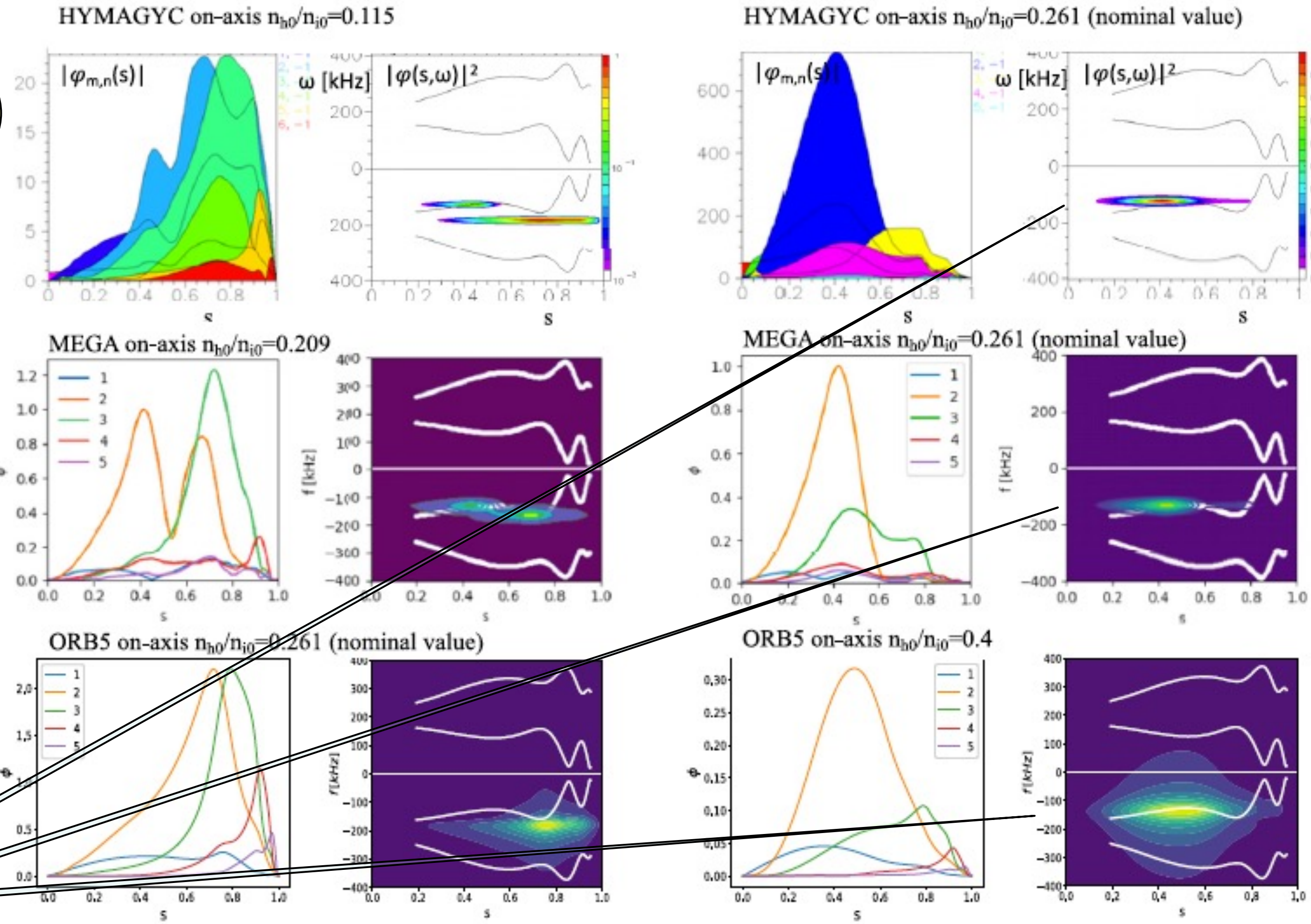
Energetic particle n_H scan for on-axis EP density profile-2

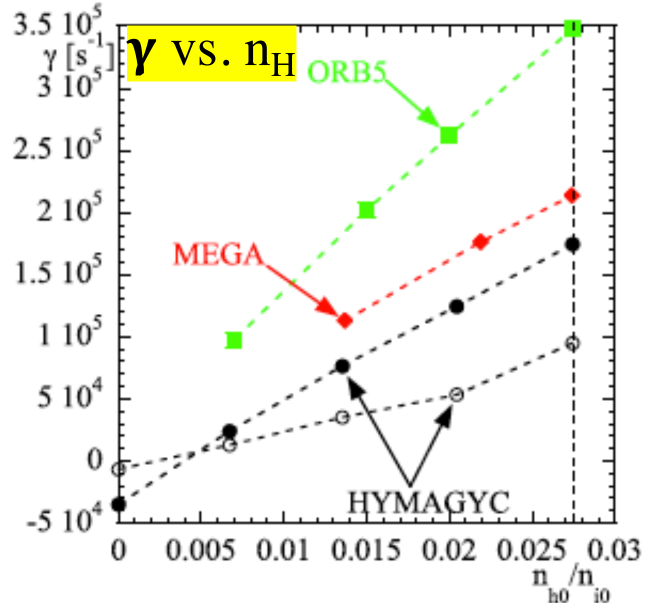


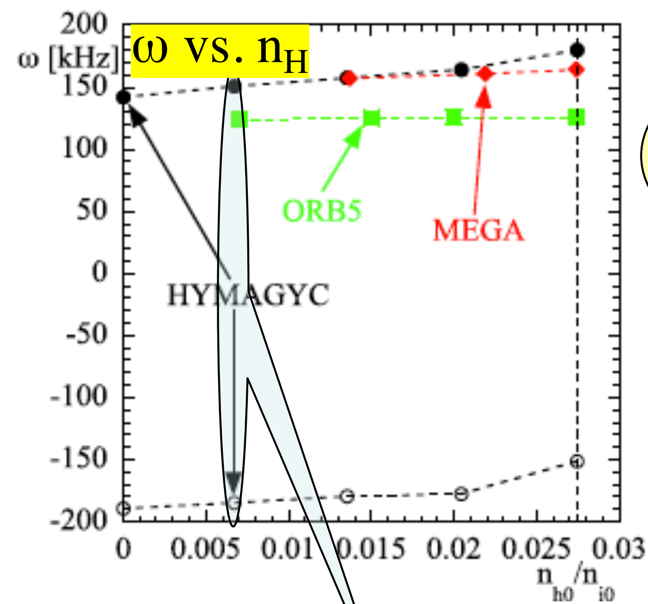


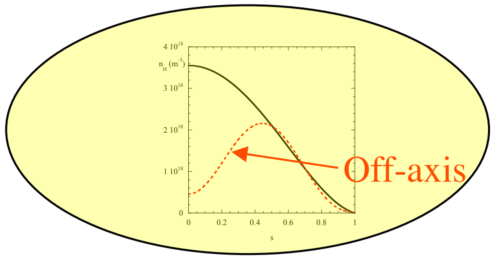




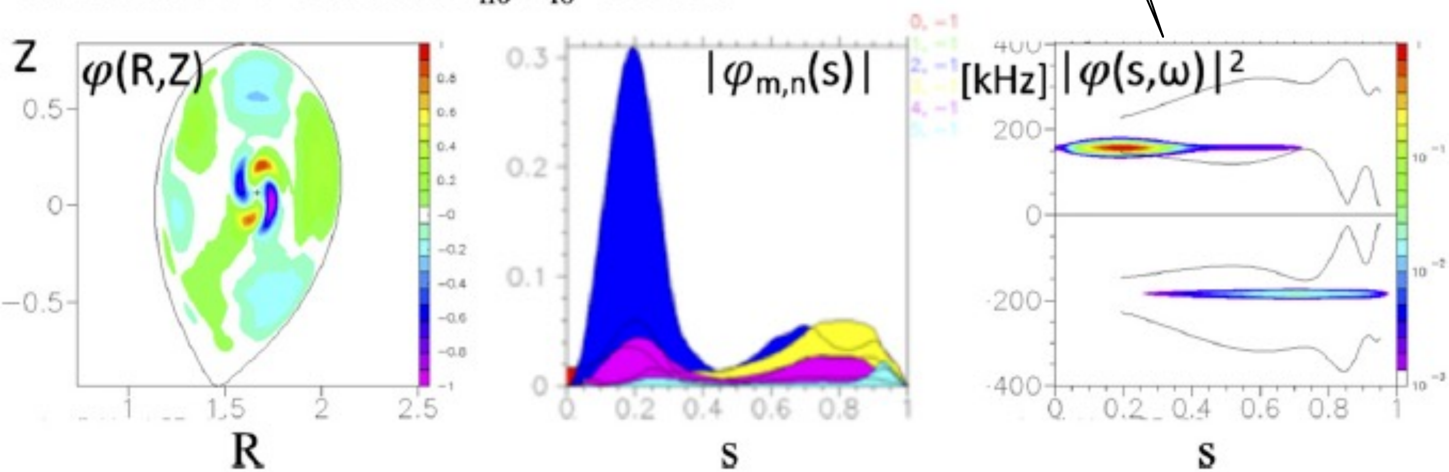
Energetic particle n_H scan for off-axis EP density profile







HYMAGYC off-axis n_{h0}/n_{i0}=0.0067



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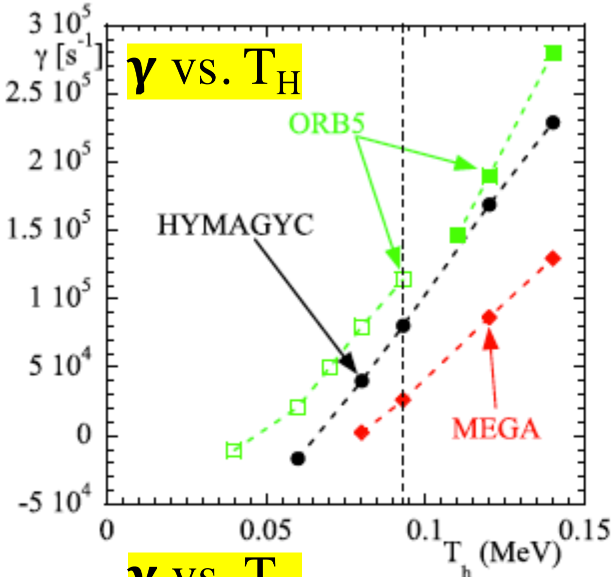
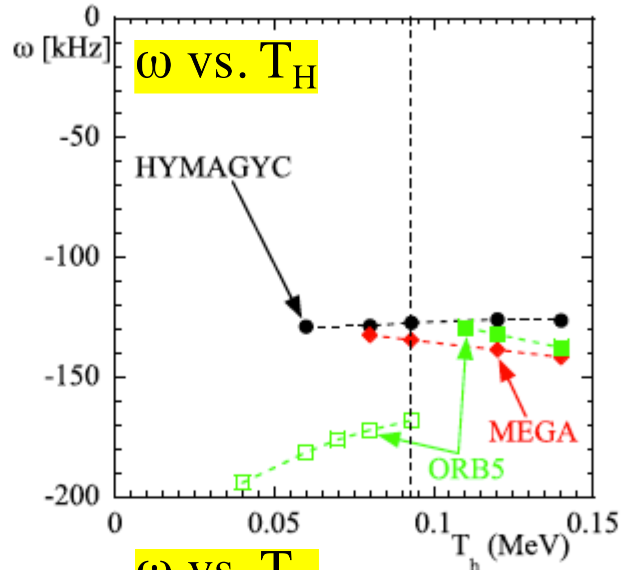
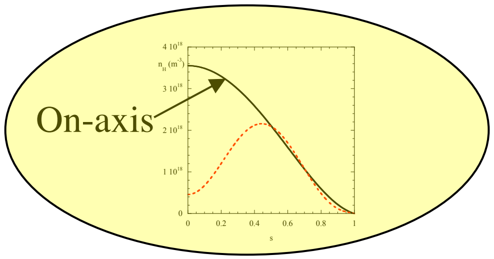
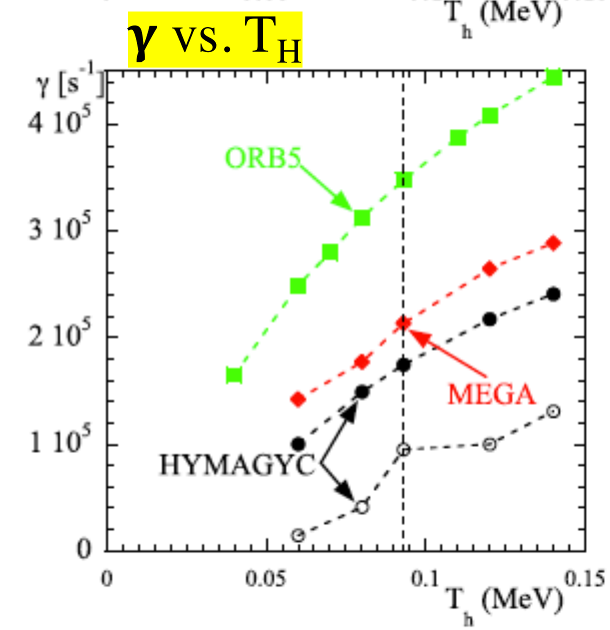
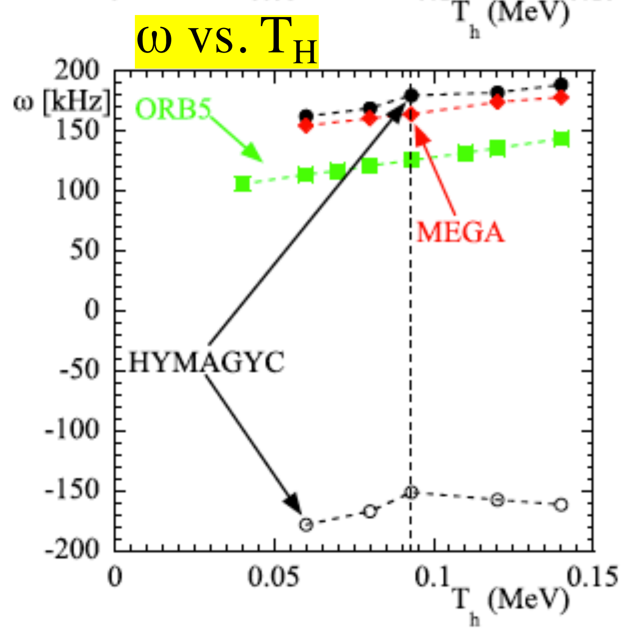
Energetic particle T_H scan for on-axis and off-axis EP density profiles

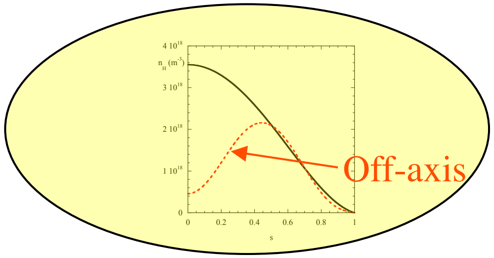








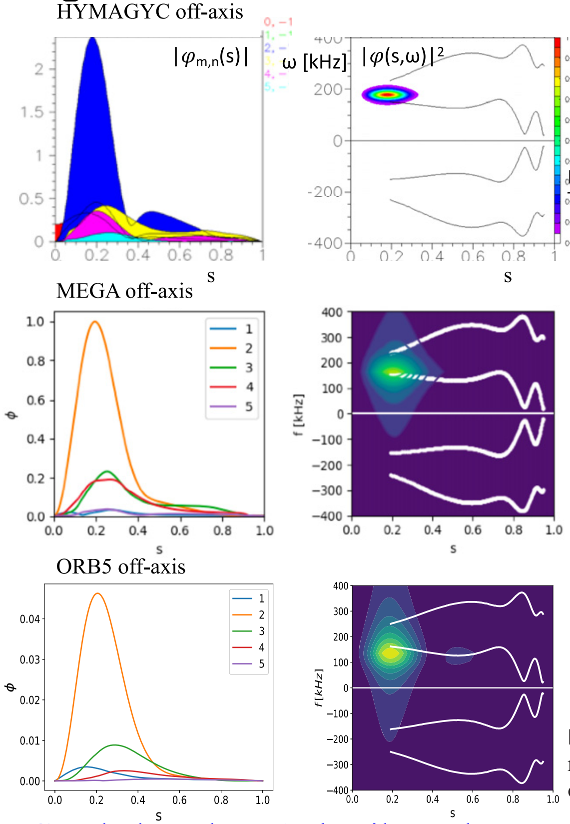




Fusion Unit EUROfusion

Non-linear benchmark

- Following the results of the linear benchmark for the AUG-NLED case, between HYMAGYC, MEGA and ORB5 (see G. Vlad et al., Nuclear Fusion, 61:116026, 2021) we analyze the nonlinear saturation of the n=-1 toroidal mode
- We compare the results of nonlinear simulations for the off-axis EP density profile case, for which all the three codes show a similar results during the linear phase: same dominant mode, i.e., very similar radial eigenfunction, real frequencies in very good agreement, growth-rate within a factor two:



[Linear phase results from: G. Vlad et al., Nuclear Fusion, 61:116026, 2021]

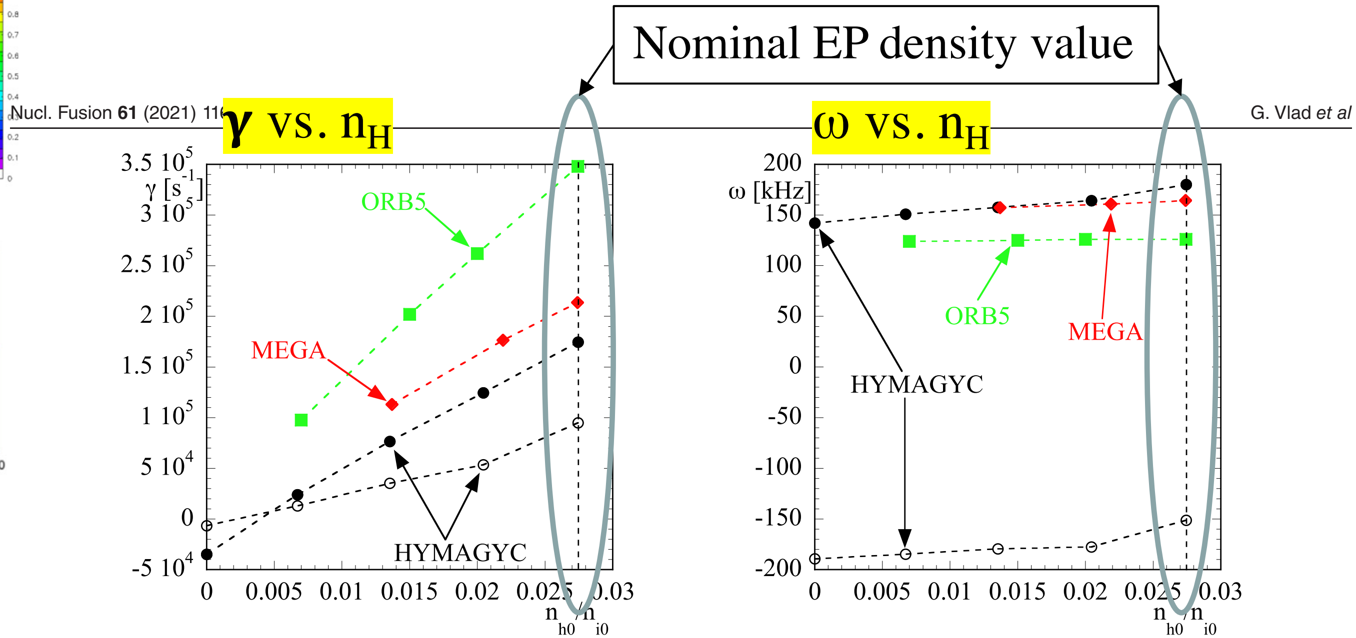
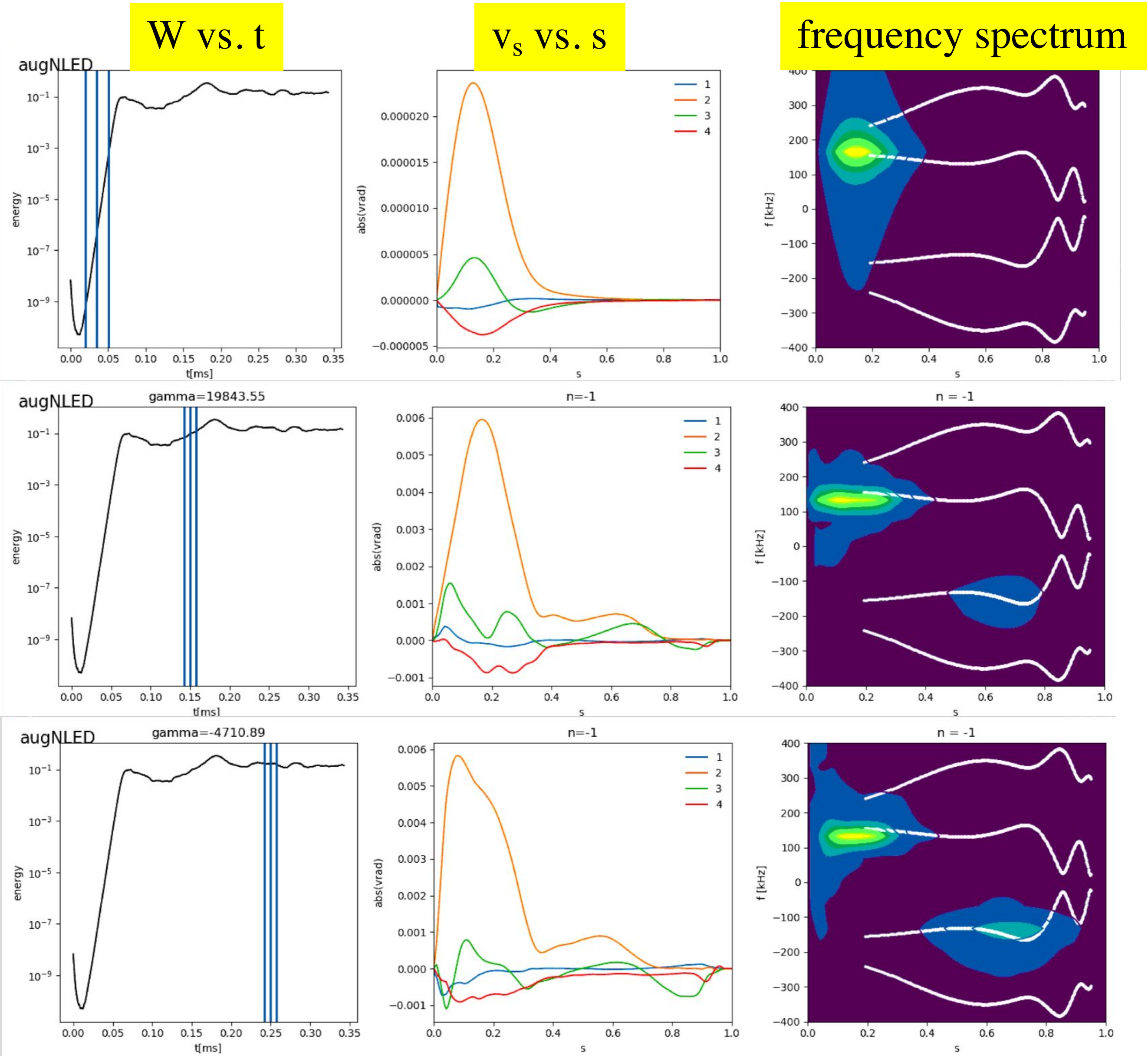


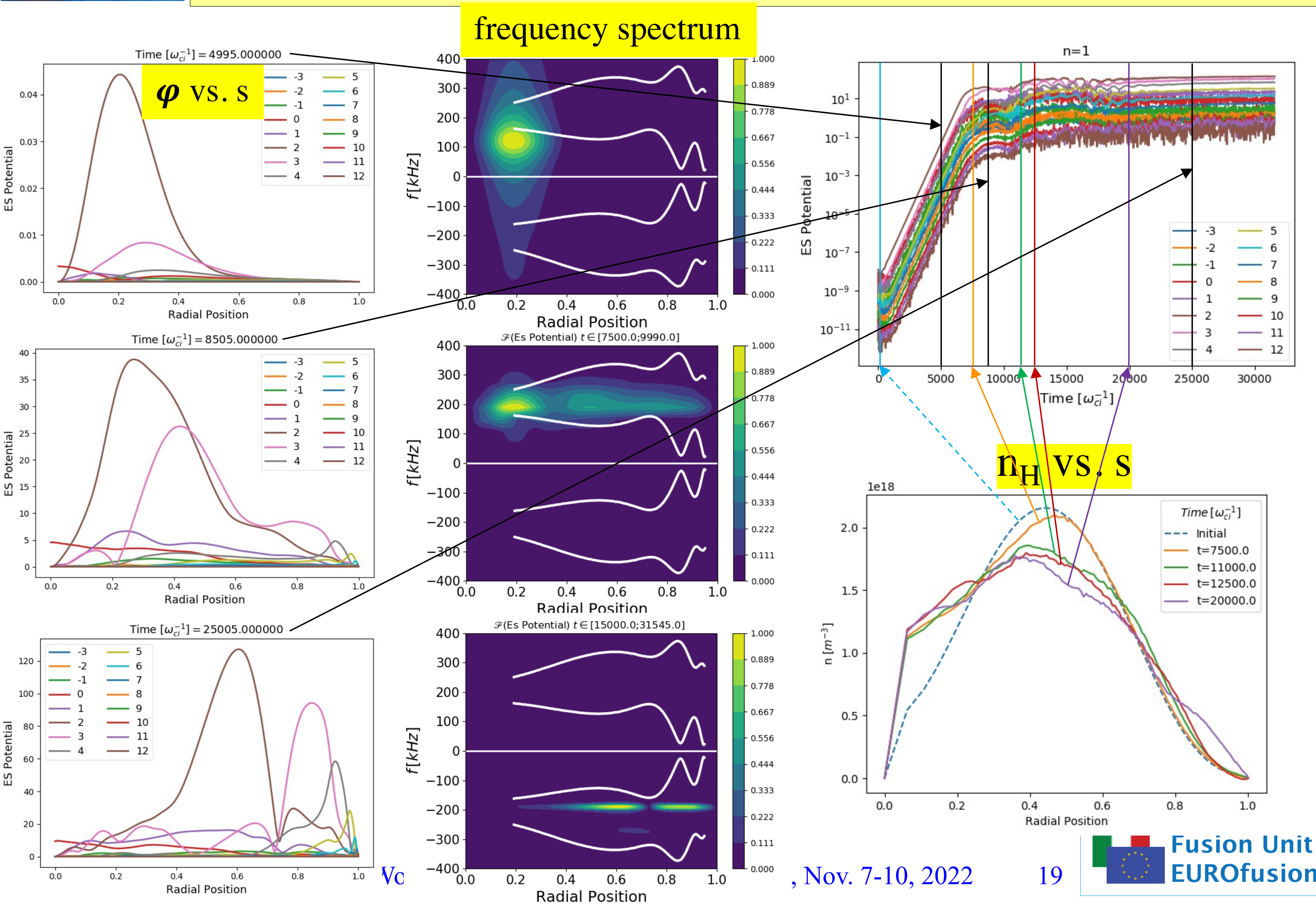
Figure 12. EP density scan for the AUG off-axis EP density profile: growth rates (left frame) and frequencies (right frame). Black circles refer to HYMAGYC results, red diamonds to MEGA, and green squares to ORB5, with closed symbols indicating core-localized TAEs and open symbols the external TAEs. The dashed black vertical lines refer to the nominal value of n_{h0}/n_{i0}.

Non-linear benchmark - MEGA



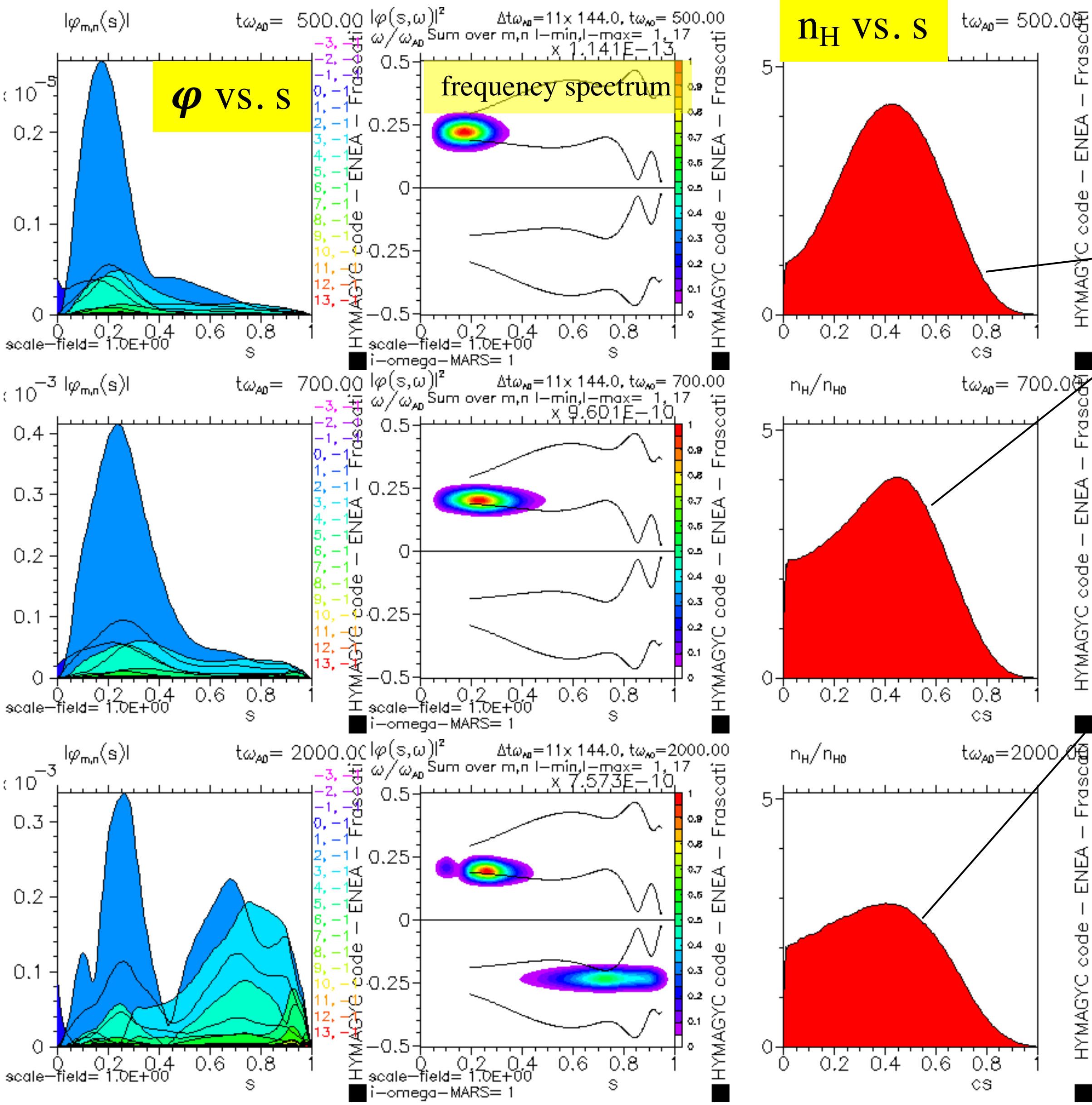
- MEGA shows the linear mode, located close to the magnetic axis, with positive real frequency
- later on, after saturation, a second, subdominant mode emerges toward the edge, with negative real frequency (i.e., rotating in the poloidal plane with opposite frequency w.r.t. the most unstable mode during linear phase)
- Note that the innermost mode is located in a radial region where the EP density gradient is positive, whereas the outermost mode is located in a radial location where the EP density gradient has opposite sign.

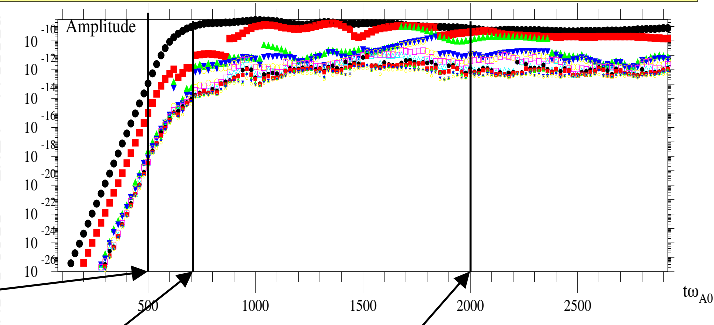
Non-linear benchmark – ORB5



Fusion Unit EUROfusion

Non-linear benchmark – HYMAGYC

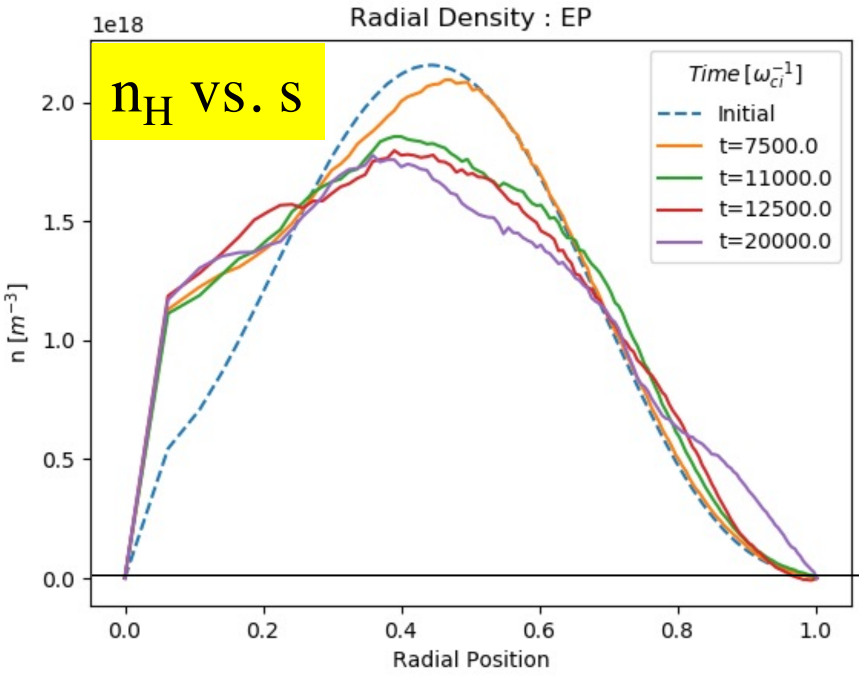




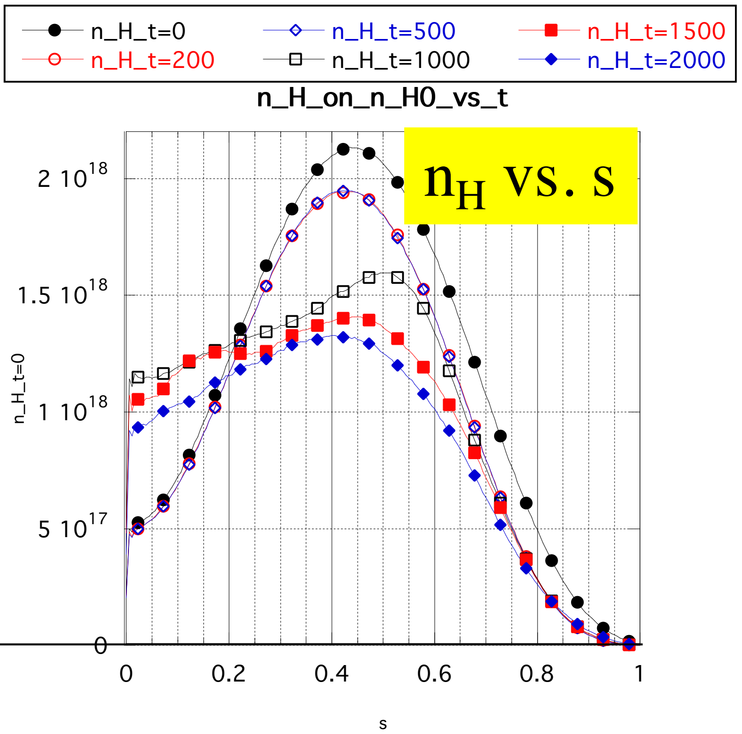
- HYMAGYC, similarly to MEGA and ORB5, shows, during the linear phase, the most unstable mode located close to the magnetic axis, with positive real frequency.
- During nonlinear saturation, a second, subdominant mode appears close to the edge, rotating in opposite direction.
- Saturation leads to "fill" the energetic particle density profile in the innermost region of the radial profile.
- Results shown are from a simulation including FLR effects; FOW simulations show similar results but more noisy...

Energetic particle density profile

ORB5



HYMAGYC



Conclusions

- Benchmark between HYMAGYC, MEGA and ORB5
- Realistic equilibrium: the fully shaped NLED-AUG test case
- Two variants of EP density profile (the peaked on-axis and the peaked off-axis ones) have been analyzed, n=1 mode considered
- Purely MHD spectra have been compared between the codes: results in good agreement
- Linear EP driven modes:
  - a remarkable agreement is observed among the three codes for the peaked off-axis case
  - when considering the peaked on-axis case, HYMAGYC and MEGA observe, as the most unstable mode, an RSAE localized around mid-radius, whereas ORB5 observes an externally localized TAE
  - varying consistently either the EP density or the temperature while keeping constant the radial profiles, i.e., by varying either n_{h0} or T_{h0}, allows to reconcile the discrepancy observed for the nominal, peaked on-axis EP density profile results.
- Preliminary comparison for nonlinear saturation benchmark shows qualitative agreement, in particular regarding the time evolution of the EP radial density profile

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[2] Aymar R. et al. 1997, FEC 1996, IAEA, Vol. 1, p.3

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Miscellanea

Careful survey of conventions used in the three codes, e.g.:

- conventions for equilibrium:
  - Grad-Shafranov signs, definition of the flux function ψ => COCOS number!
- conventions for Fourier transforms (space, time):
  - HYMAGYC, e.g., uses:
    - for space variables: $$v^s(s,\chi,\phi) = e^{in\phi} \sum_{m=m_1}^{m_2} v^s_m(s)\, e^{im\chi}$$
    - for Fourier transform in time (following the usual linear MHD convention, such that $\gamma>0$ corresponds to growing modes, with $\omega=\omega_0+i\gamma$): $f(t) = \mathrm{int}[f(\omega) \exp(-i\, \omega\, t)\, d\omega]$
  - different definitions of various quantities and normalizations (e.g., ω_{A0}, B_0, B_{geo}, $B_{mag.\ axis}$, $B_{vacuum/plasma}$, resistivity, etc.)

- To avoid this kind of questions, it would be very useful to work in the same environment (as, e.g., ITMENV, IMAS, ...)

  => HYMAGYC is "almost itmenv/imasenv" compliant

MEGA description

Standard MHD equations

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \boldsymbol{v}) + \nu_{\mathrm{n}} \Delta(\rho - \rho_{\mathrm{eq}}), \quad (1)$$

$$\rho \frac{\partial}{\partial t}\boldsymbol{v} = -\rho \vec{\omega} \times \boldsymbol{v} - \rho \nabla \left(\frac{v^2}{2}\right) - \nabla p + (\boldsymbol{j} - \boldsymbol{j}_h') \times \boldsymbol{B} + \frac{4}{3}\nabla(\nu \rho \nabla \cdot \boldsymbol{v}) - \nabla \times (\nu \rho \vec{\omega}), \quad (2)$$

$$\frac{\partial \boldsymbol{B}}{\partial t} = -\nabla \times \boldsymbol{E}, \quad (3)$$

$$\frac{\partial p}{\partial t} = -\nabla \cdot (p \boldsymbol{v}) - (\gamma - 1) p \nabla \cdot \boldsymbol{v} + (\gamma - 1)[\nu \rho \omega^2 + \frac{4}{3}\nu\rho(\nabla \cdot \boldsymbol{v})^2 + \eta \boldsymbol{j} \cdot (\boldsymbol{j} - \boldsymbol{j}_{\mathrm{eq}})] + \chi \Delta(p - p_{\mathrm{eq}}), \quad (4)$$

$$\boldsymbol{E} = -\boldsymbol{v} \times \boldsymbol{B} + \eta(\boldsymbol{j} - \boldsymbol{j}_{\mathrm{eq}}), \quad (5)$$

$$\boldsymbol{j} = \frac{1}{\mu_0}\nabla \times \boldsymbol{B}, \quad (6)$$

$$\vec{\omega} = \nabla \times \boldsymbol{v}, \quad (7)$$

- In the MEGA code, the bulk plasma is described using nonlinear MHD equations, and the energetic ions are simulated with both the full-f and δf particle method.
- The energetic ion contribution is included in the MHD momentum equation [Eq. (2)] as the energetic ion current density $\boldsymbol{j}_h'$ that includes the contributions from parallel velocity, magnetic curvature and gradient drifts, and magnetization current. The $\boldsymbol{E} \times \boldsymbol{B}$ drift disappears in $\boldsymbol{j}_h'$ owing to quasi-neutrality. The electromagnetic field is given by the **standard MHD** description. The MHD equations are solved using a fourth-order in the space and time finite-difference scheme.
- The **drift-kinetic** description is employed for the alpha particles in current simulations.
- Current MEGA MHD solver is also extended using **an extended MHD model given by Hazeltine and Meiss.**

ORB5 description

- ORB5[1] is a global, nonlinear, gyrokinetic, electromagnetic, PIC code which can take into account collisions and sources.
- The Vlasov-Maxwell gyrokinetic equations are derived through variational principles from a gyrokinetic Lagrangian. Field equations are derived via functional derivatives.
- The distribution function is discretized through numerical particles (markers). The fields are discretized through cubic B-splines.
- The gyrokinetic model of ORB5 contains the reduced MHD as subset[2].

[1]E. Lanti et al., "ORB5: A global electromagnetic gyrokinetic code using the PIC approach in toroidal geometry". In: Computer Physics Communications (2019).
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