EUROfusion

Numerical tools for burning plasma applications

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Content

- Software stack under development at the TSVV Task 10

  (EUROfusion's E-TASC project) is presented.

- Major projects requiring the HPC resources are the global gyrokinetic codes ORB5 and EUTERPE.

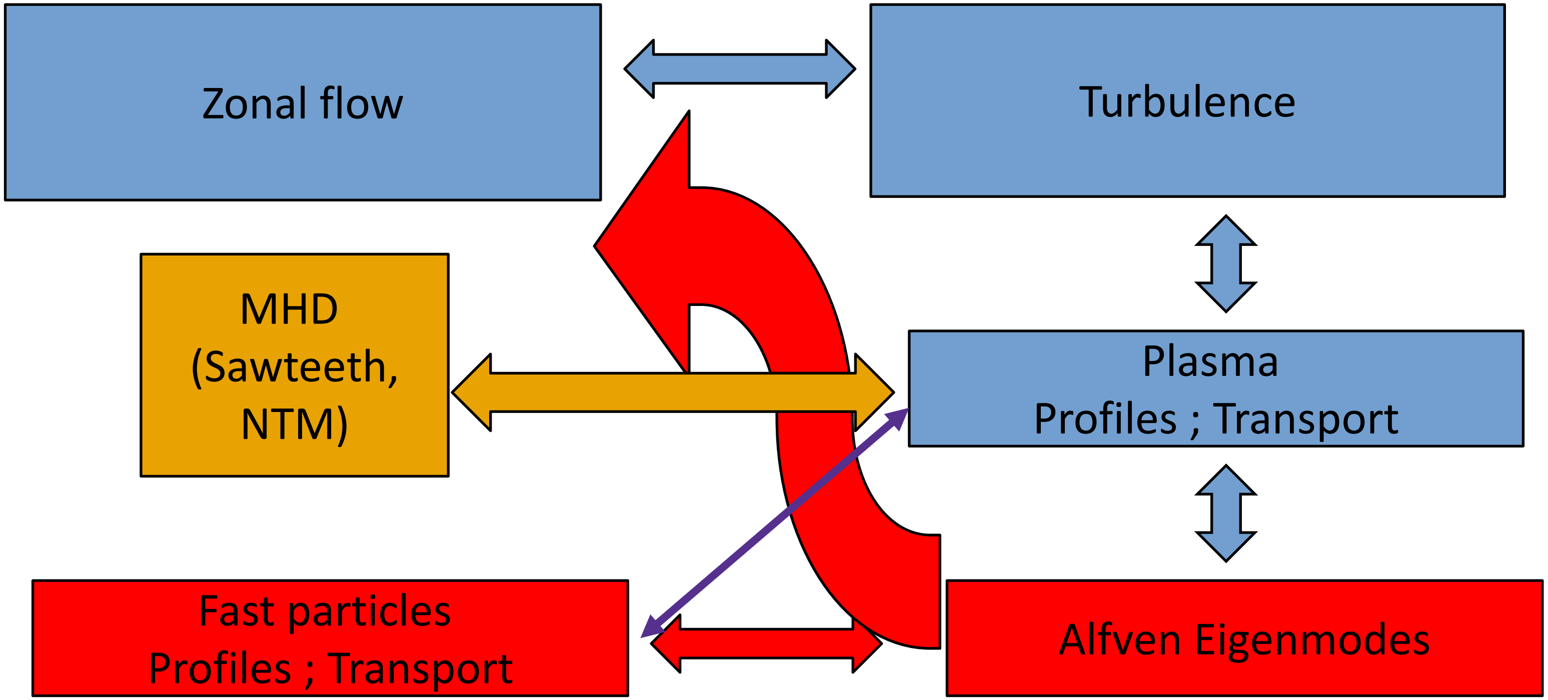
- For longer time scales (e.g. sawtooth cycle), global hybrid-MHD codes HYMAGYC and XTOR can be used.

- Integrated modeling tools include IMAS-based Energetic-Particle Workflow and SCENIC framework (radio-frequency heating and fast-ion generation).

- Basic models employed are described and simulation examples are shown.

System couplings in burning plasmas

- Energetic Particles (EP) are abundant in burning plasmas
- „Meso-scale“ EP dynamics introduces couplings across scales



Single framework

- Burning plasmas will have high beta and include energetic particles
- Presence of energetic particles creates complex coupled system
- Single framework including all parts consistently is needed
- Many parts of the problem are kinetic and global
- Many connections between the parts are kinetic and global
- **Global gyrokinetic approach** is a minimal inclusive description
- Global gyrokinetics requires intensive computation (exa-scale)
- Reduced models can be used to speed-up computations

hybrid kinetic-MHD, **reduced EP models**, **integrated modeling**

Major actors and topics of interest:

Energetic particle orbits, global Alfvénic and MHD modes, shear Alfvén continuum, avalanches, profile corrugations, phase-space structures (holes/clumps), reconnection/turbulence, Alfvén Eigenmodes-zonal flows-turbulence, ...

Gyrokinetic equations (mixed variables)

https://doi.org/10.1088/1361-6587/ac0bcb

The equations include the gyrokinetic Vlasov equation:

$$\frac{\partial f_{1s}}{\partial t} + \dot{\boldsymbol{R}} \cdot \frac{\partial f_{1s}}{\partial \boldsymbol{R}} + \dot{v}_\parallel \frac{\partial f_{1s}}{\partial v_\parallel} = -\dot{\boldsymbol{R}}^{(1)} \cdot \frac{\partial F_{0s}}{\partial \boldsymbol{R}} - \dot{v}_\parallel^{(1)} \frac{\partial F_{0s}}{\partial v_\parallel} \ , \tag{1}$$

the equations for the gyro-center orbits:

$$\dot{\boldsymbol{R}} = \dot{\boldsymbol{R}}^{(0)} + \dot{\boldsymbol{R}}^{(1)} \ , \quad \dot{v}_\parallel = \dot{v}_\parallel^{(0)} + \dot{v}_\parallel^{(1)} \tag{2}$$

$$\dot{\boldsymbol{R}}^{(0)} = v_\parallel \boldsymbol{b}_0^* + \frac{1}{qB_\parallel^*} \boldsymbol{b} \times \mu \nabla B \ , \quad \dot{v}_\parallel^{(0)} = -\frac{\mu}{m} \boldsymbol{b}_0^* \cdot \nabla B \tag{3}$$

$$\dot{\boldsymbol{R}}^{(1)} = \frac{\boldsymbol{b}}{B_\parallel^*} \times \nabla \left\langle \phi - v_\parallel A_\parallel^{(\mathrm{s})} - v_\parallel A_\parallel^{(\mathrm{h})} \right\rangle - \frac{q}{m} \langle A_\parallel^{(\mathrm{h})} \rangle \, \boldsymbol{b}_0^* \tag{4}$$

$$\dot{v}_\parallel^{(1)} = -\frac{q}{m} \left[\boldsymbol{b}^* \cdot \nabla \left\langle \phi - v_\parallel A_\parallel^{(\mathrm{h})} \right\rangle + \frac{\partial}{\partial t} \left\langle A_\parallel^{(\mathrm{s})} \right\rangle \right] - \frac{\mu}{m} \frac{\boldsymbol{b} \times \nabla B}{B_\parallel^*} \cdot \nabla \left\langle A_\parallel^{(\mathrm{s})} \right\rangle \tag{5}$$

$$\boldsymbol{b}^* = \boldsymbol{b}_0^* + \frac{\nabla \langle A_\parallel^{(\mathrm{s})} \rangle \times \boldsymbol{b}}{B_\parallel^*} \ , \quad \boldsymbol{b}_0^* = \boldsymbol{b} + \frac{m v_\parallel}{q B_\parallel^*} \nabla \times \boldsymbol{b} \tag{6}$$

$$B_\parallel^* = B + \frac{m v_\parallel}{q} \boldsymbol{b} \cdot \nabla \times \boldsymbol{b} \ , \tag{7}$$

Field equations:

$$-\nabla \cdot \left(\frac{n_0}{B \omega_{ci}} \nabla_\perp \phi \right) = \bar{n}_{1i} - \bar{n}_{1e}$$

$$\frac{\partial}{\partial t} A_\parallel^{(\mathrm{s})} + \boldsymbol{b} \cdot \nabla \phi = 0 \ ,$$

$$\sum_{s=i,e} \frac{\beta_s}{\rho_s^2} A_\parallel^{(\mathrm{h})} - \nabla_\perp^2 A_\parallel^{(\mathrm{h})} = \mu_0 \sum_{s=i,e} \bar{j}_{\parallel 1s} + \nabla_\perp^2 A_\parallel^{(\mathrm{s})}$$

Gyrokinetic particle-in-cell codes

- "Klimontovich" representation for perturbed distribution function:

$$\delta f_s(\boldsymbol{R}, v_\parallel, \mu, t) = \sum_{\nu=1}^{N_p} w_{s\nu}(t)\delta(\boldsymbol{R} - \boldsymbol{R}_\nu)\delta(v_\parallel - v_{\nu\parallel})\delta(\mu - \mu_\nu) \ ,$$

- Maxwellian distribution for all species:

See talk of T. Hayward-Schneider for non-Maxwellian F_{0s}

$$F_{0s} = n_0 \left(\frac{m}{2\pi T_s}\right)^{3/2} \exp\left[-\frac{m_s v_\parallel^2}{2T_s}\right] \exp\left[-\frac{m_s v_\perp^2}{2T_s}\right]$$

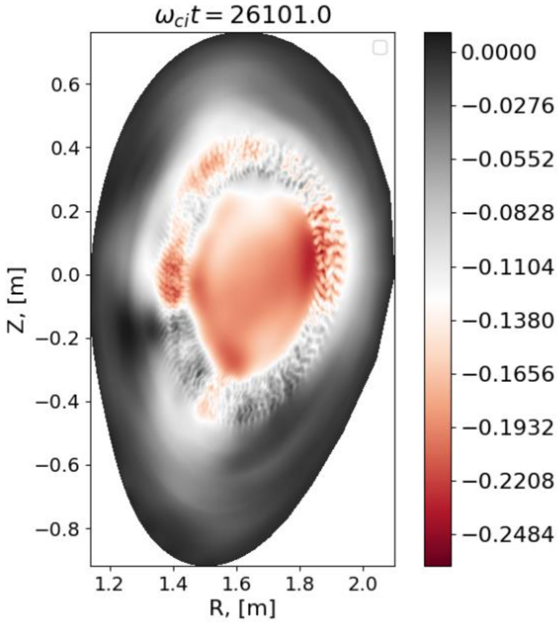
- Finite-element discretization for fields:

$$\phi(\boldsymbol{x}) = \sum_{l=1}^{N_s} \phi_l(t)\Lambda_l(\boldsymbol{x}) \ , \quad A_\parallel(\boldsymbol{x}) = \sum_{l=1}^{N_s} a_l(t)\Lambda_l(\boldsymbol{x}) \ ,$$

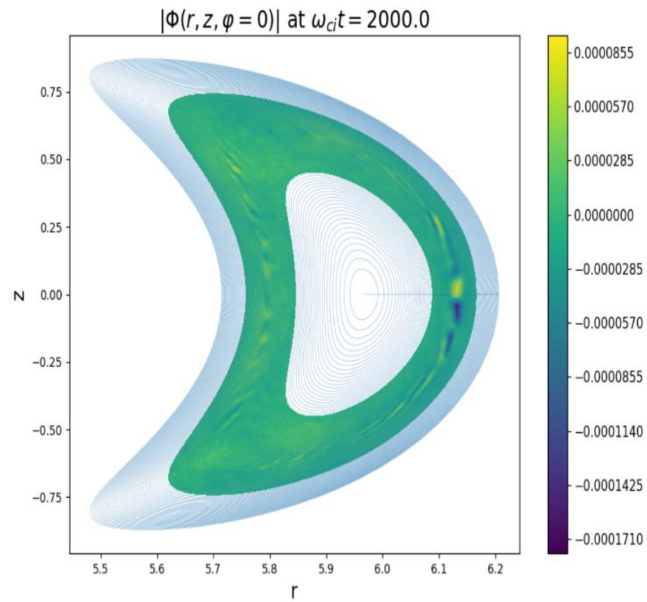
- Larmor structure for GPU-enabling in ORB5; OpenACC
- GPU-enabling of EUTERPE: separate routines for different particle species; openacc, now transitioning to OpenMP 5.x (wider support, more architectures)
- Replacing „globals“ (global data) with Fortran abstract types
- Gradual transition of the code base (EUTERPE) to C++
- General trend in computing
- Better access to accelerator frameworks (such as Kokkos)

Global gyrokinetic EM turbulence (ORB5/EUTERPE)

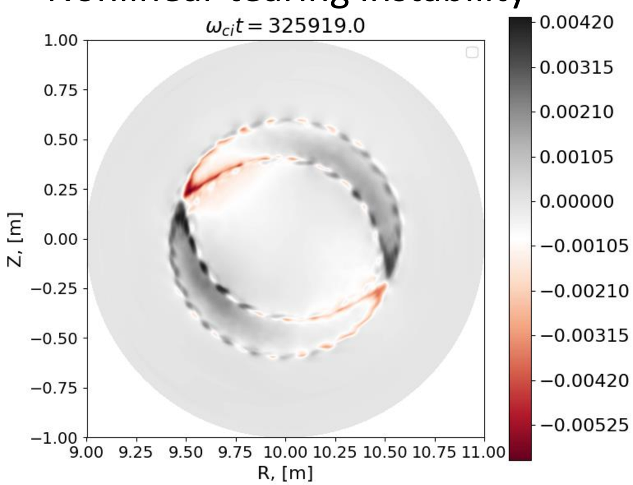
KBM turbulence in ASDEX-U



EM turbulence in W7-X



Nonlinear tearing instability



Extensions to other physics (meso-/micro-scale couplings):

(1) Tearing instability: interaction with EM turbulence

(2) Alfvenic (e.g. TAEs) + fast ions + EM turbulence (ITGs) + ZF

Global EM turbulence in ASDEX-U and W7-X

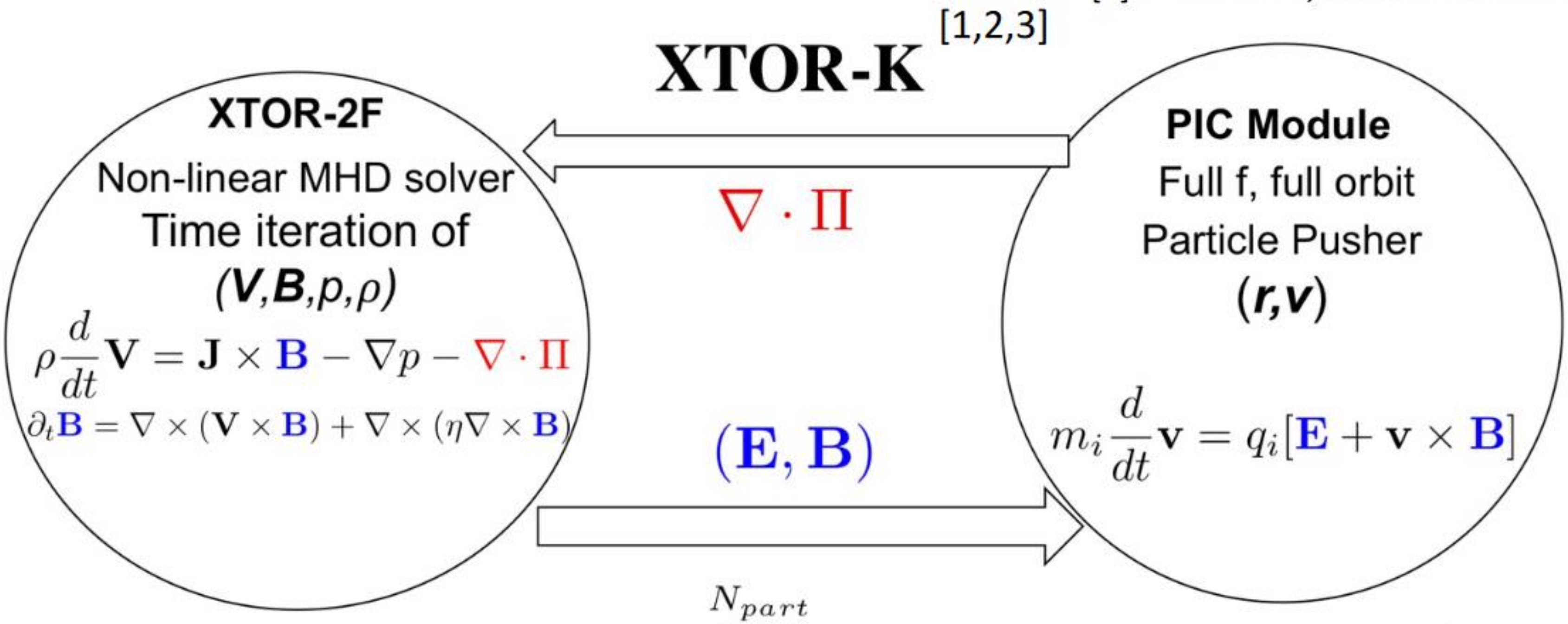
(1) Numerically accessible on existing HPC

(2) Detailed physics studies and algorithmic improvements ongoing

(3) Extensions to other machines (e.g. JET, TCV) desirable

Nonlinear kinetic-MHD hybrid code XTOR-K

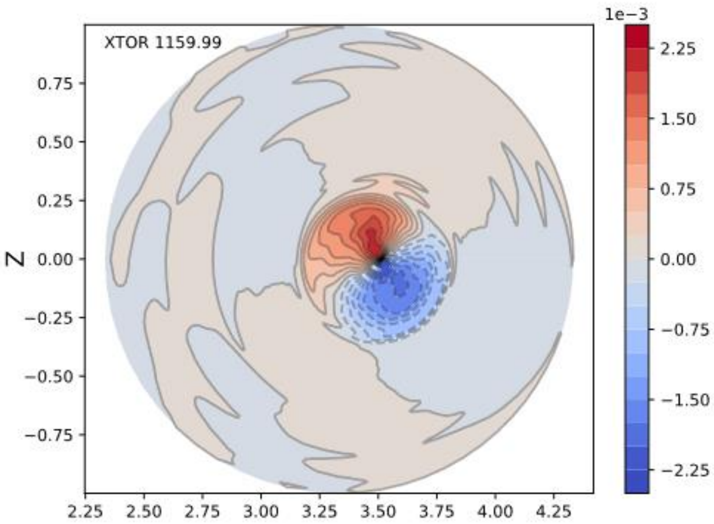
[1] *H. Lütjens et al, JCP 2010*
[2] *D. Leblond, PhD thesis 2013*
[3] *G. Brochard, PhD thesis 2019*



$$\Pi(\mathbf{r}, t) = m_i \sum_{n=1}^{N_{part}} \mathbf{v}_n \mathbf{v}_n \delta(\mathbf{r} - \mathbf{r}_n(t))$$

j

Internal Kink simulations:
hybrid simulation with 2 Mev Fusion alphas

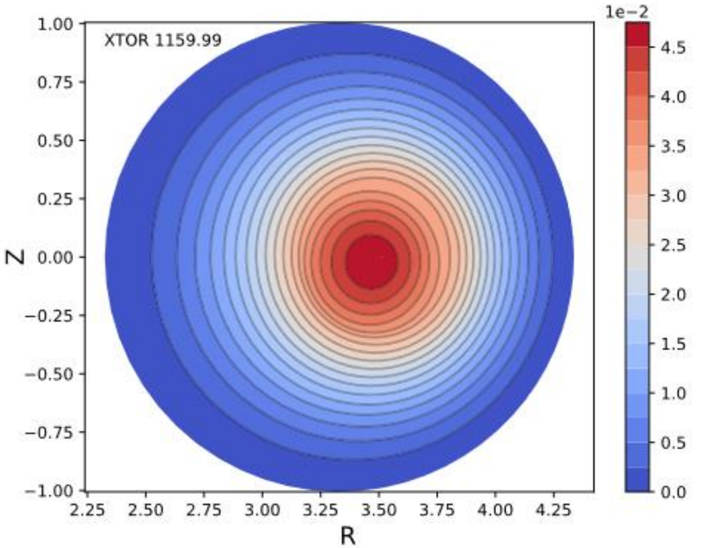


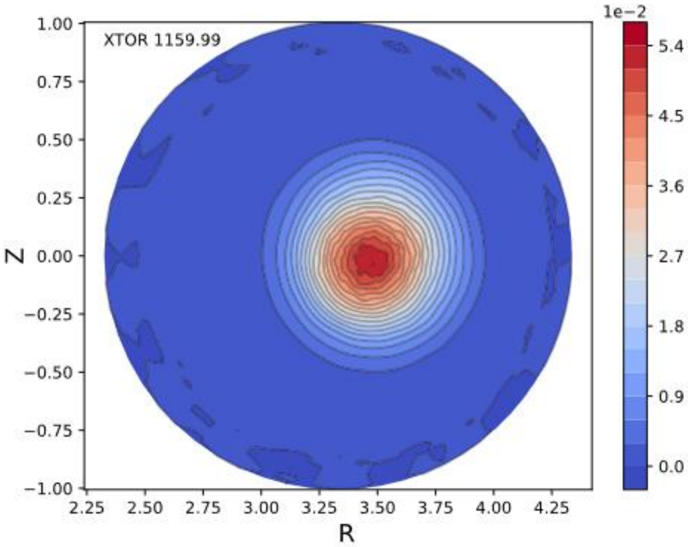
V_r(phi=0)

Ni0=ne0=2 10^19 m-3
Ti0=Te0=30KeV
Nf0=4.10^17 m-3
Beta_pol=0.78;
r(q=1)=0.45
S=3.e6
Chi//=1., Chi_perp=1.e-6

saturated kink regime

Fluid and kinetic ion pressures





HYMAGYC

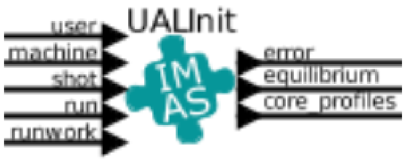
- HYMAGYC is a hybrid MHD-gyrokinetic code to study energetic particles and Alfvénic instabilities

- Arbitrary tokamak equilibria (e.g. from CHEASE)

- Thermal (core) plasma described by linear full resistive MHD equations (MARS transformed to initial value code)
- Energetic particle described by nonlinear gyrokinetic equation
- Fully-nonliner gyrokinetic contribution enters via pressure tensor in momentum equation

- HYMAGYC is a highly IMASified code

Progress in using HYMAGYC with IMAS-IDSs



UALInit actor - Universal Access Layer Initializator:

- open the Database, extract the required IDSs (equilibrium, core_profiles,…) and passes to the next actor

hymagycimas actor:

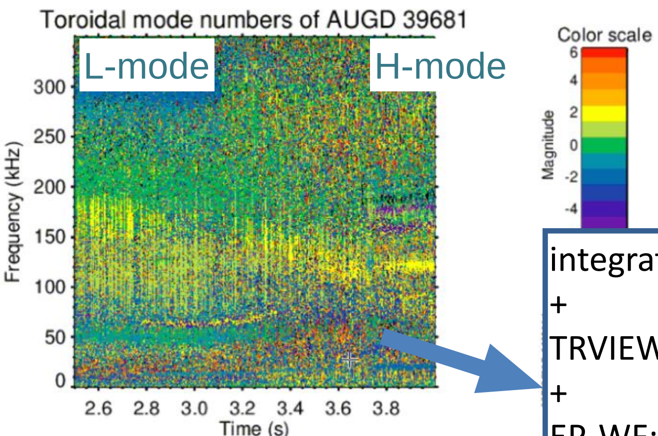
- it contains the actual code HYMAGYC prepared to receive the input data from the IMAS database;
- Code parameters entered via xml files;
- It transforms the input data to the actual data required by HYMAGYC to run (e.g., equilibrium geometry, metric tensor coefficients, initial conditions, change COCOS conventions, normalizations, etc.);
- Execute the Job;
- Forward the final output to the UALSliceCollector.

UALSliceCollector actor - Universal Access Layer actor

- Writes the output data to the Database;
- Close the Database.

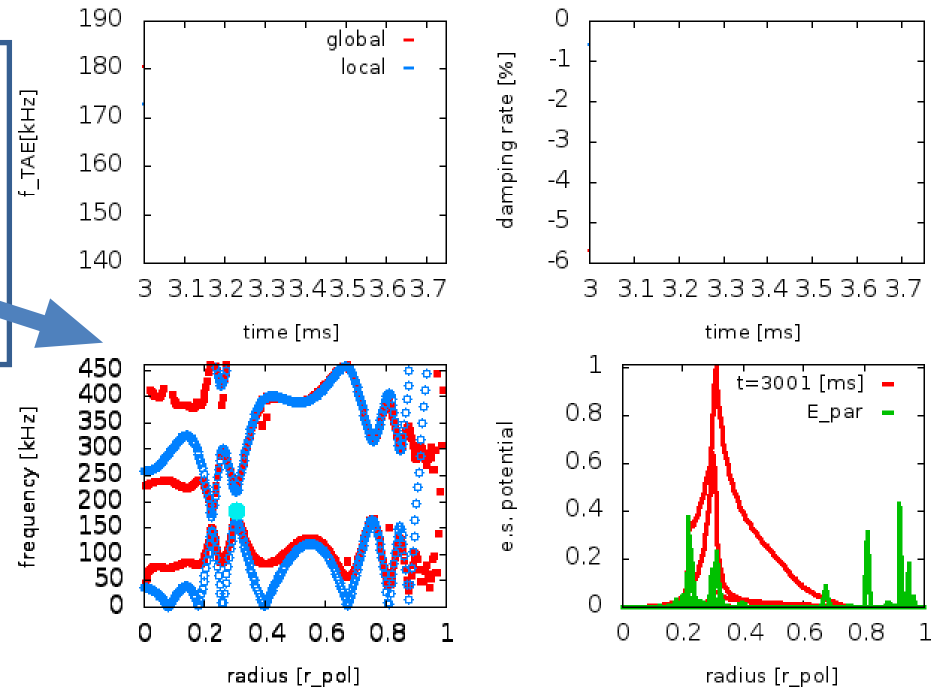
Energetic-particle Workflow (LIGKA)

linear stability: GK code LIGKA has been evolved into automated stability workflow (EP-WF)
AUG data example: L-H transition in presence of n=2 TAE



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

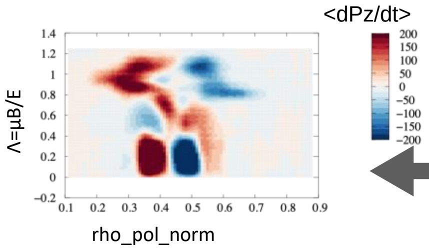
integrated data analysis
+
TRVIEW(IMAS interface)
+
EP-WF: LIGKA local
+
EP-WF: LIGKA global



- analyse L-mode,H-mode and transition phases:
beat infamous problem of AE stability sensitivity to profiles - compare trends instead of single time slices
- compare local and global models
- systematic uncertainty quantification feasible
- applied also to TCV, JET, JT-60SA, ITER

Energetic-particle Workflow (transport)

reduced models to describe EP transport:
solve transport equations for phase space zonal structures (Eurofusion ENR ATEP)

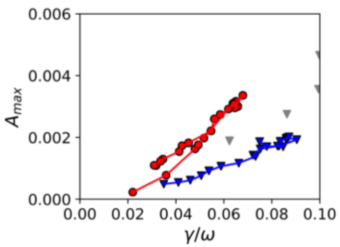


calculate PSZS

ATEP code: solve transport equation for PSZS with sources and collisions

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

[M. Falessi 2017-2022]



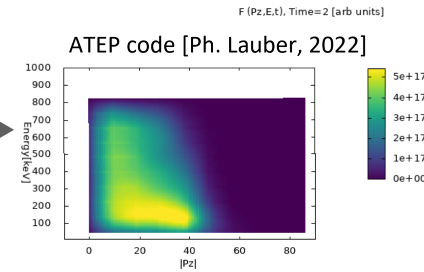
use
NL code/model
for intensity closure

calculate
D(r,E)

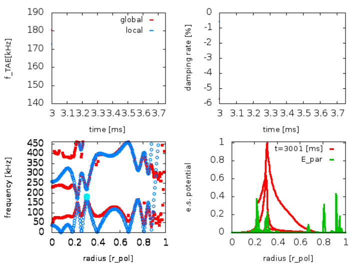
or

advance
F_{EP}
and return
updated
distribution IDS,
or its moments

ATEP code [Ph. Lauber, 2022]



EP WF (LIGKA)



calculate
linear mode
spectrum

can be extended to include zonal structures
driven by turbulence and their mutual interaction

t

t+1

core_transport
equilibrium
mhd_linear
distributions

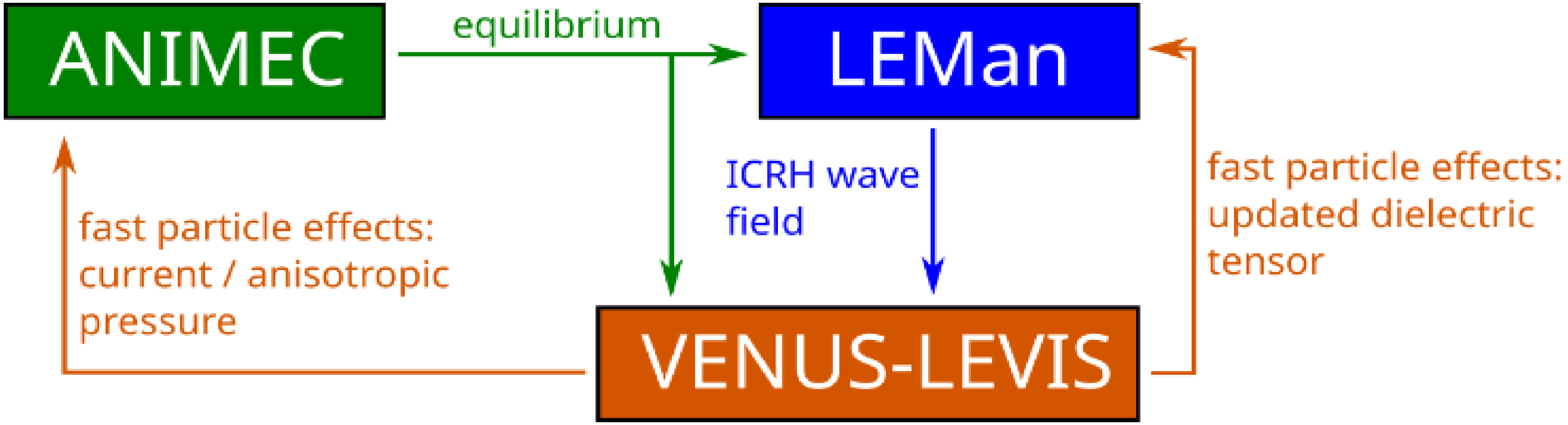
transport code

time

distributions

The SCENIC code package

- SCENIC[1] is now run in Greifswald to model ICRH physics
- iterative procedure of three (coupled) codes
- usually 5 – 10 iterations necessary to find consistent solution
  - ANIMEC (anisotropic equilibrium)
  - LEMan (full-wave code / plasma enters with its dielectric tensor)
  - VENUS-LEVIS (particle following in the ICRH wave field / Monte-Carlo kicks)



adapted from M. Machielsen

SCENIC computes EP distribution function which can be used by other codes

[1] M. Jucker et al., Comm. Phys. Commun. 183, 912-925 (2011)

Conclusions

- **Burning plasma are complex multiscale system**
- **Coupling electromagnetic turbulence and zonal flows =>**
- **=> Energetic particles and Alfven Eigenmodes =>**
- **=> Alfven Eigenmodes and zonal flows in presence of MHD activity**
- **Global gyrokinetic theory includes all system components**
- **Particle-in-cell codes can be used to simulated burning plasmas**
- **For long-time dynamics, model reduction is necessary**
- **Hybrid-MHD for sawtooth cycles, fishbone bursts, etc.**
- **Integrated modelling for discharge time scale (Energetic-Particle Workflow)**
- **Integrated modelling for heating**

Enabling factors:

(1) improvements in theory and simulation algorithms

(2) code optimization and extension to accelerators (GPUs etc.)

(3) strong increase in computing resources and experimental data

BACK-UP

XTOR-K fluid equations

$$\partial_t\left(\sum_{s=i,k} m_s n_s \mathbf{u}_s\right) = \mathbf{J}\times\mathbf{B} - \sum_{s=i,e}\nabla p_s - \sum_{s=i,e}\nabla.\mathbf{\Pi_s} - \sum_k \nabla.\mathbf{P_k} = 0$$

$$\partial_t \mathbf{B} = -\nabla\times\mathbf{E}$$

$$\mathbf{E} = -\mathbf{v}\times\mathbf{B} - \frac{1}{en_e}\hat{\mathbf{b}}(\hat{\mathbf{b}}.\nabla p_e)) + \frac{\mathbf{J}_\parallel}{\sigma_\parallel} + \frac{\mathbf{J}_\perp}{\sigma_\perp}$$

$$\partial_t n_i = -\nabla.\left(n_i(\mathbf{v}+\mathbf{v}_i^*) - D_\perp\nabla n_i + D_\perp \nabla n_{i,0}\right)$$

$$\frac{DS_s}{Dt} + \frac{\nabla.\mathbf{Q}_s}{p_s} = 0$$

$$S_s = \ln\frac{T_s^{1/(\Gamma-1)}}{n_s} = \frac{1}{\Gamma-1}\ln\frac{p_s}{n_s^\Gamma}, \text{ and } \mathbf{Q}_s = \frac{5}{2}\frac{p_s}{q_s}\frac{\mathbf{B}}{B^2}\times\nabla T_s$$

$$n_e = Z_i n_i + \sum_k Z_k n_k$$

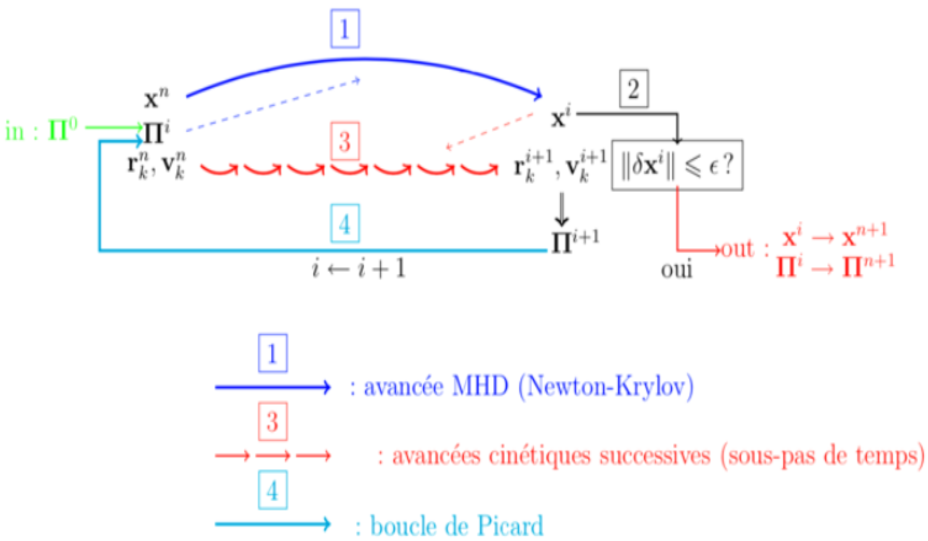
$$D/Dt = \partial_t + \mathbf{u}_s.\nabla$$

$$\mathbf{u}_s = \mathbf{v}_{s,\parallel} + \mathbf{v}^{(1)}_{\perp,s} + \mathbf{v}^{(2)}_{\perp,s}$$

$$\mathbf{v}_{s,\parallel} = v_{s,\parallel}\hat{\mathbf{b}} = (\hat{\mathbf{b}}.\mathbf{u}_s)\hat{\mathbf{b}}$$

$$\mathbf{v}^{(1)}_{\perp,s} = \frac{\mathbf{E}\times\mathbf{B}}{B^2} + \frac{\mathbf{B}\times\nabla p_s}{n_s q_s B^2}$$

XTOR-K: hybrid scheme



- MHD advance: pre-conditioned Newton Krylov (iterative). Inherited from XTOR-2F (JCP-2010). Physical pre-conditioner
- Kinetic ion advance: Boris Buneman PIC
- Unconditionnaly stable for fluid time steps of interest

Last year:

- Pre-conditioning with a parallel SPIKE-LU solver
- Merge into the hybrid kinetic/fluid environment of the code.
- Newton Krylov using petsc DD features: ready for other families of pre-conditioners (mathematical)

Gains:

- Factor 2 due to particle sorting (reduces strongly cash missings for moment depositions)
- Factor 2.5 due to the new solver

→ Overall factor of 5 in cpu time and much better global parallelization properties

NLED ASDEX-Upgrade EP benchmark

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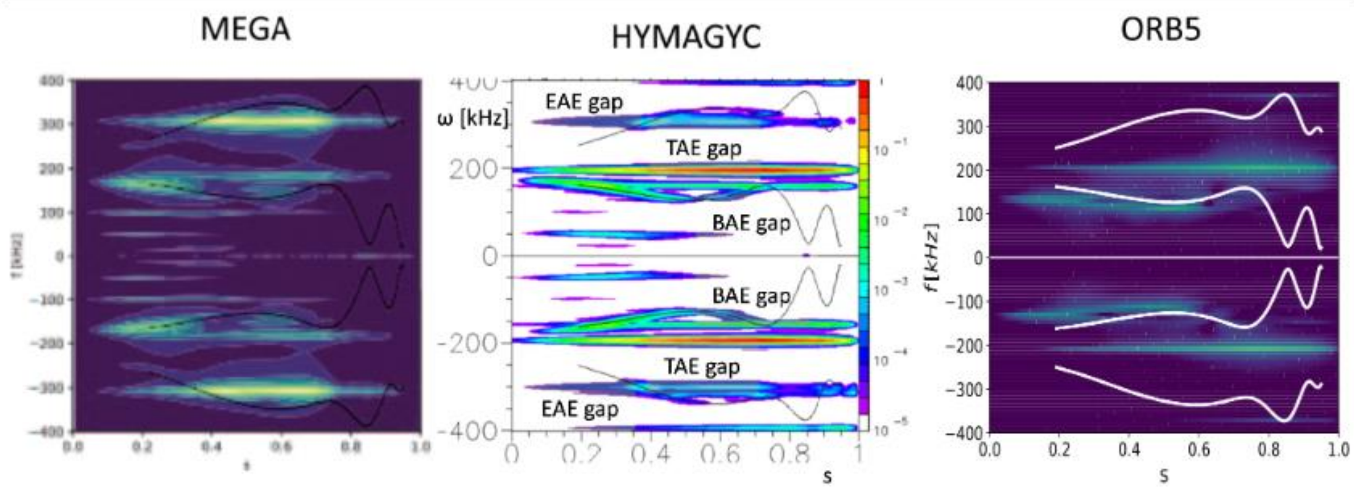

Figure 6. Frequency spectra in the MHD limit for MEGA (left), HYMAGYC (centre), and ORB5 (right). Logarithmic color scale is used for the intensity of the e.s. field $|\varphi(s,\omega)|^2$. Shear Alfvén continuous spectra are also shown using black continuous lines for the MEGA and HYMAGYC spectra, 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.

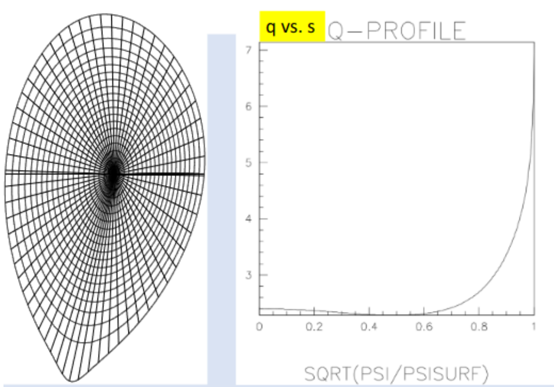

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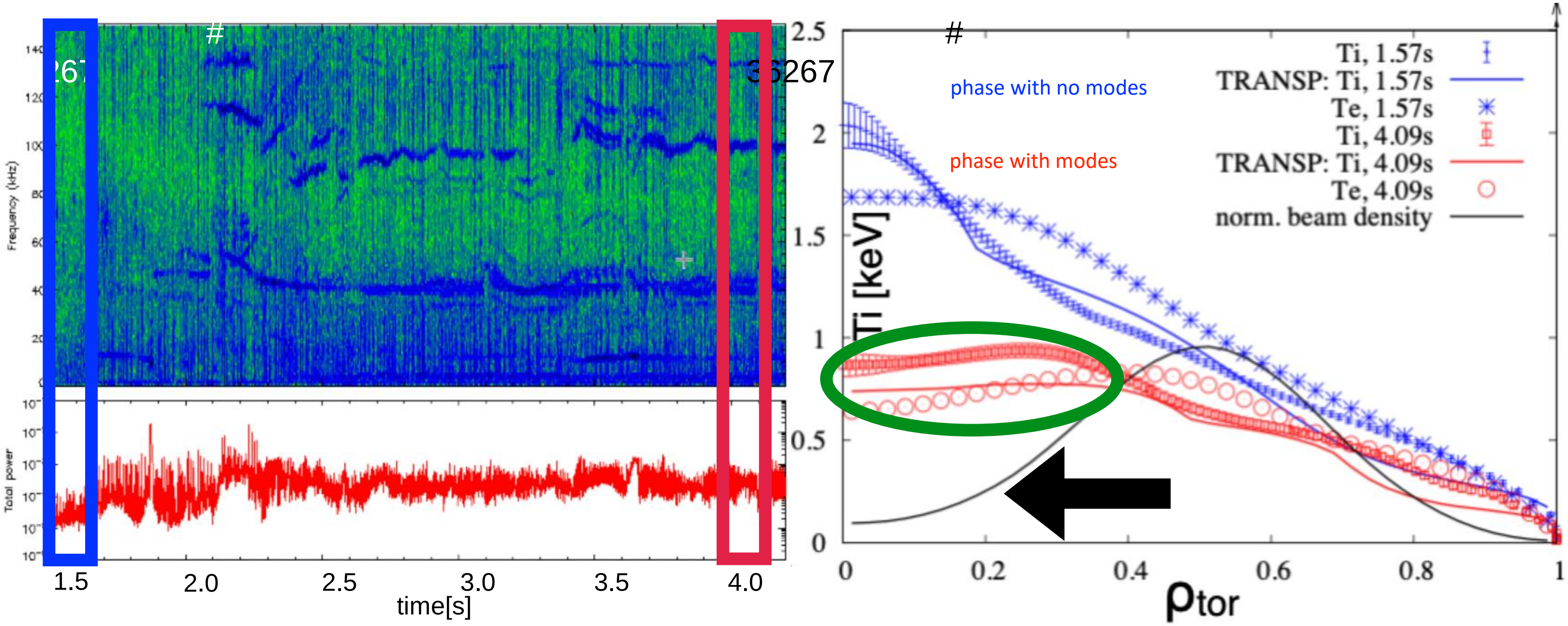
Table 4. Growth rates (s^{-1}) and real frequencies (kHz) of some of the modes observed in figure 6, corresponding to the HYMAGYC, MEGA and ORB5 purely MHD simulations, on-axis AUG reference case.

Mode	$\gamma_{\mathrm{HYMAGYC}}$ (s^{-1})	$\omega_{\mathrm{HYMAGYC}}$ (kHz)	γ_{MEGA} (s^{-1})	ω_{MEGA} (kHz)	γ^a_{ORB5} (s^{-1})	ω^a_{ORB5} (kHz)
Tearing-$q=3$	4080.2	0.0				
TAE-2	−14594.6	−159.2	−45060.0	−171.9	≈ −10000	−146
TAE-1	−6455.3	−195.8	−36057.0	−185.2	≈ −6000	−206
TAE-3	−29484.2	−301.4	−30120.0	−304.2		
EAE	−13542.3	−395.8				

Evidence for anomalous core background ion heating due to Alfvénic modes?

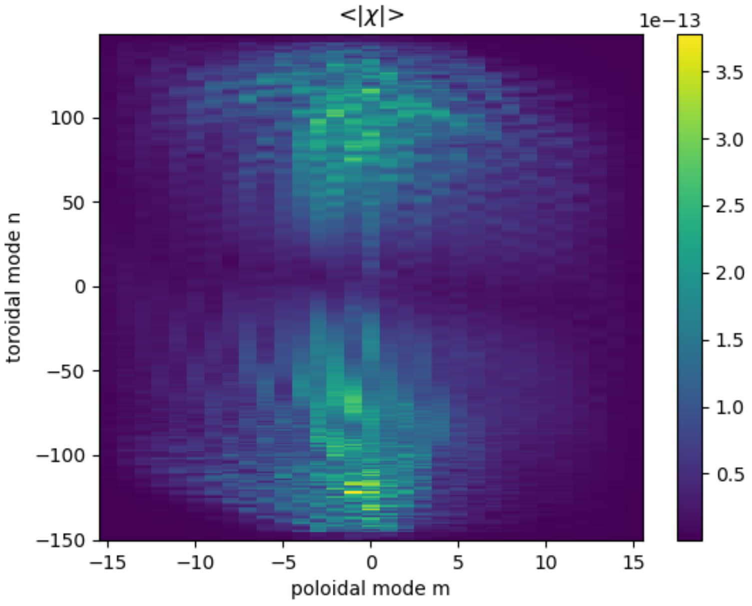
assess effect of EP re-distribution on Ti profiles - is the EP transport enough to explain the Ti difference?

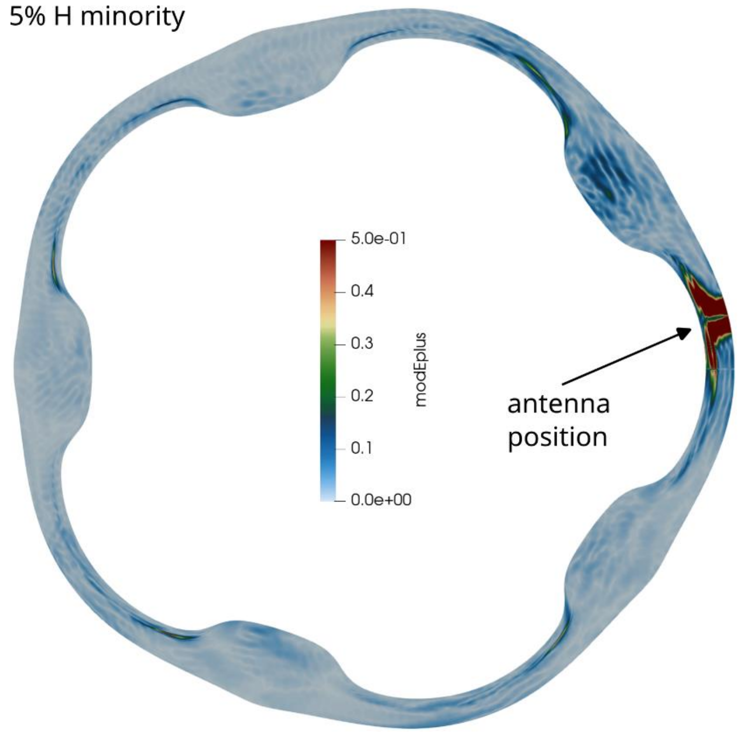


other cases/experiments very welcome - TCV, JET, JT-60SA, ITER ongoing

ICRH in W7-X: He-plasmas with H-minority

- simulations with high Fourier resolution $m \in [-15, 15]$, $n \in [-150, 149]$ have been performed
- split into 5 separate simulations (for the 5 mode families of W7-X $\rightarrow 5 \cdot 1860$ modes)





- high resolution needed to resolve small structures $\rightarrow$ realistic results

<u>SCENIC computes EP distribution function which can be used by other codes</u>