# The role of global gyrokinetic simulations in multi-scale transport modeling


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*European Science Foundation Exploratory Workshop:*

*Multi-Scale Methods For Waves And Transport Processes In Fusion Plasmas:*

*The Legacy Of Grigory Pereverzev*

Association Euratom-Tekes

# Motivation

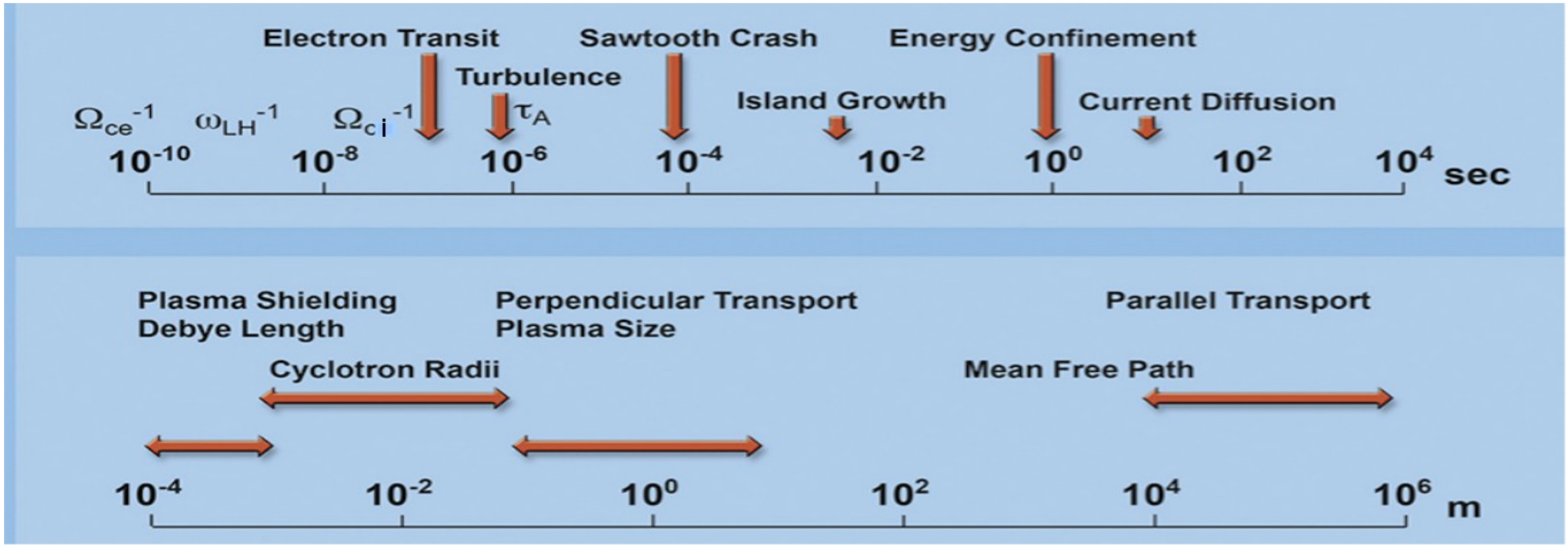
• To determine the fusion power of future machines it is necessary to accurately predict the time evolution of density, temperature and rotation profiles on an energy confinement time.

• Reduced 1D integrated transport modeling (ASTRA, TRANSP, JETTO) are used to determine the relation between profiles, sources/sinks and fluxes.

• Multiple local flux-tube simulations at different radial positions can be used to evolve the macroscopic profiles in time. But the boundary conditions and the treatment of sources & sinks can be a problem.

• Global full-f gyrokinetic simulations simultaneously evolve the fluctuations and the equilibrium in time while taking heat sources and sinks into account.---> self-consistent

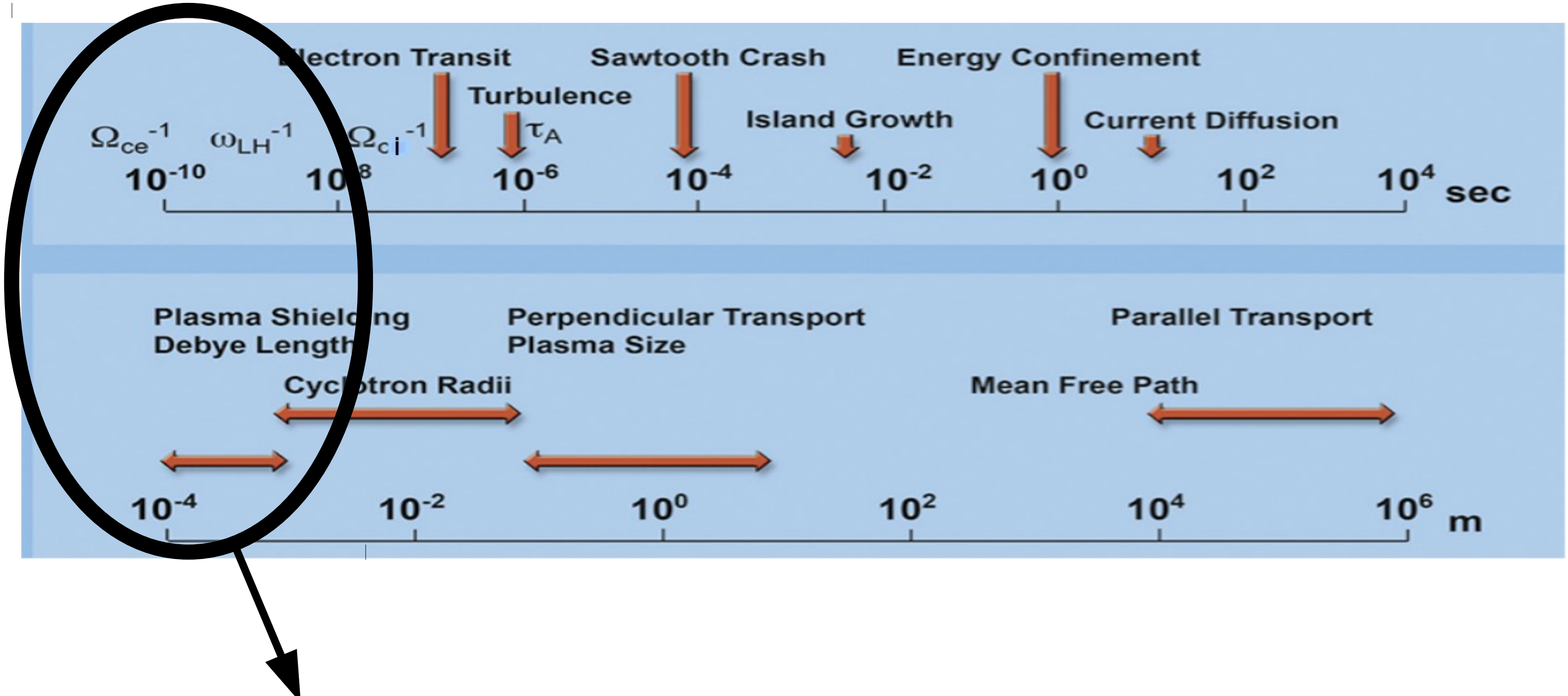
# Large scale separation in ITER plasmas




- Grid spacings ~ 3D space x 3D velocity x time

--> Multi-scale methods that use physics guidance are required

# Large scale separation in ITER plasmas




<u>Multiscale model for Collisions:</u> Relaxing the original requirement for the numbers of particles in the Debye sphere by making collisions a subgrid phenomena.

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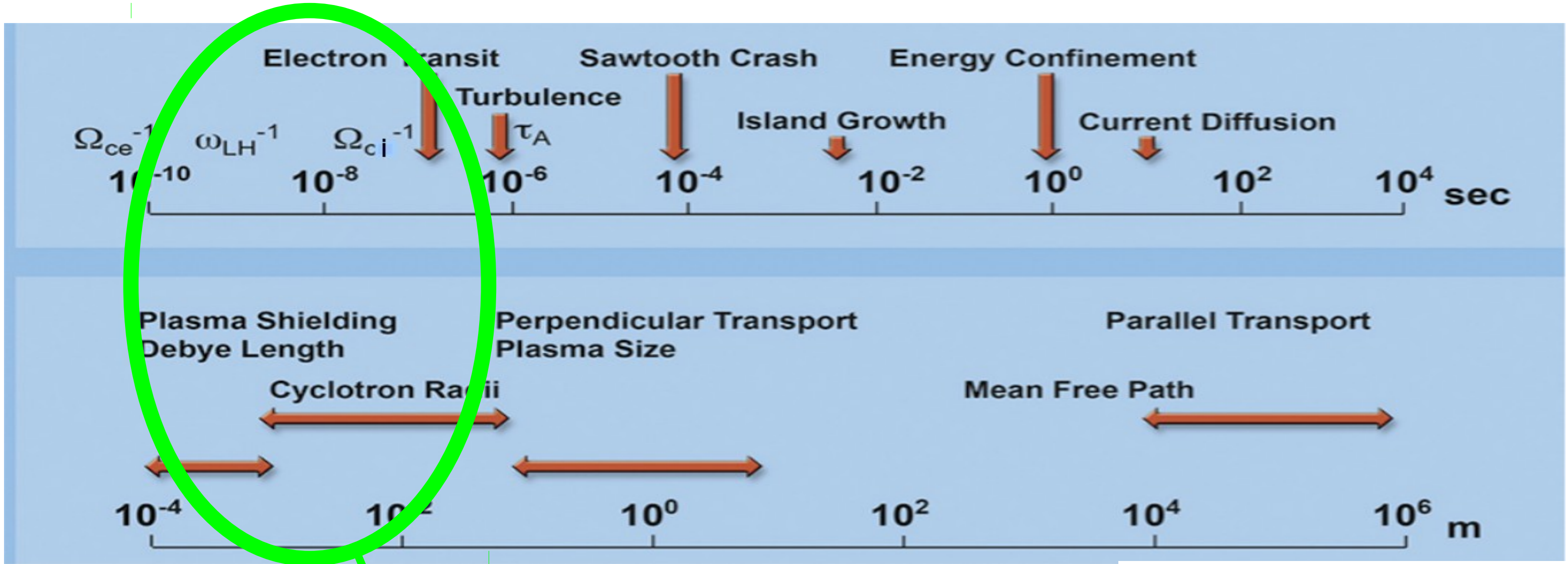
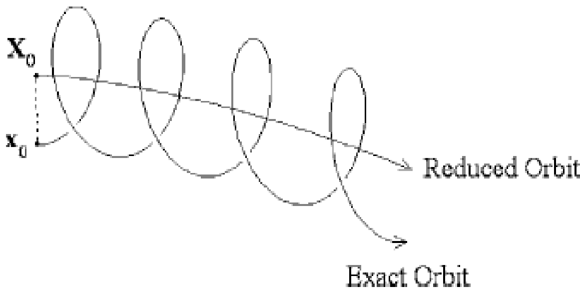



Gyrokinetic formalism eliminates the gyroangle dependency reducing the problem size from 3D to 2D in velocity space.




$$(\vec{r}, \vec{v}) \longrightarrow \left(\vec{R}, v_{\parallel}, v_{\perp}\right)$$

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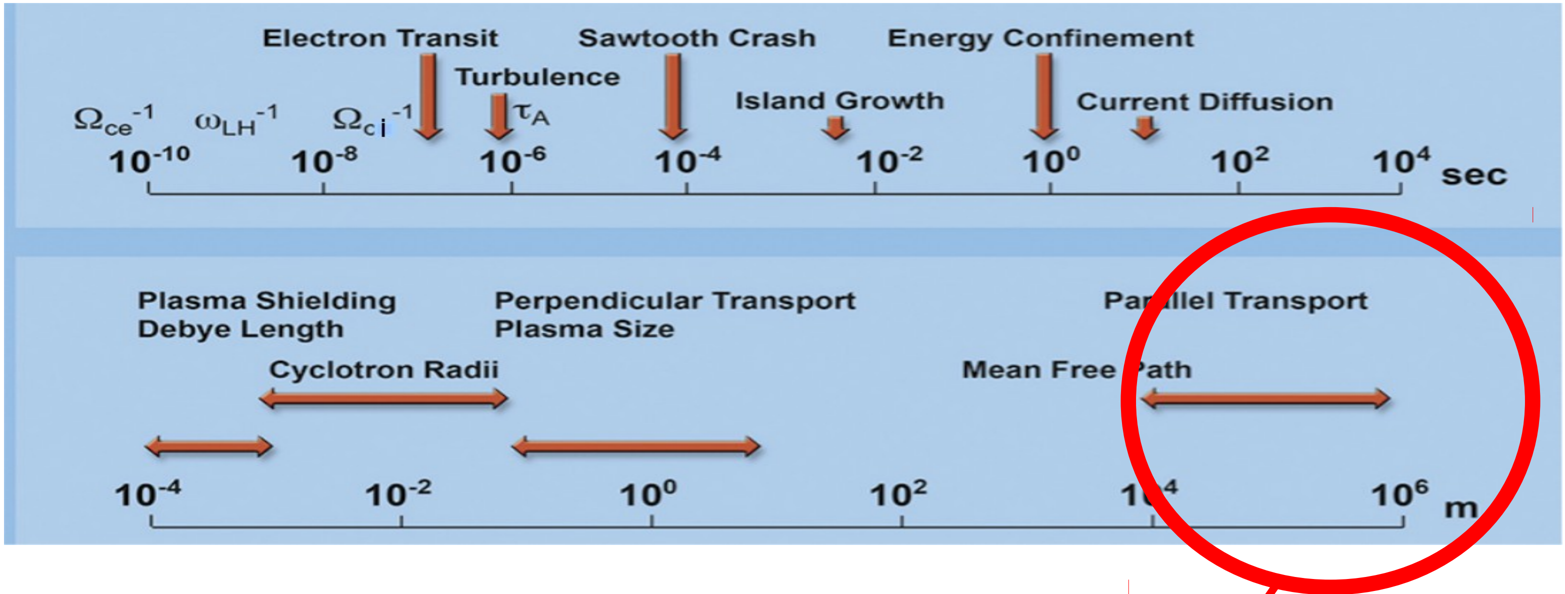
# Large scale separation in ITER plasmas




Magnetic coordinates (ψ, θ, ζ) take advantage of a k||<<k⊥ and greatly improve the computational requirements for fusion plasmas.

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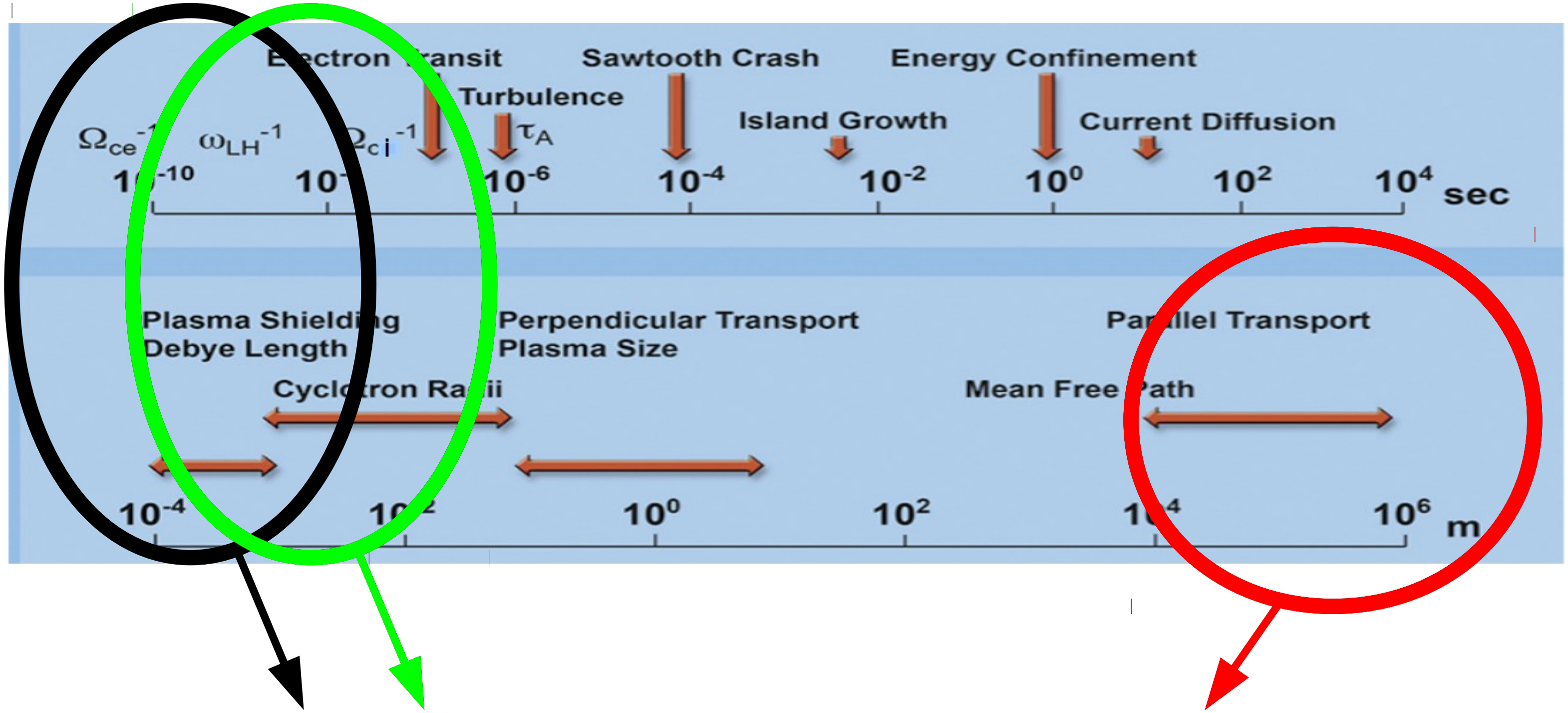
# Large scale separation in ITER plasmas




$$(L_{\parallel}/\Delta_{\parallel}) \times (L_{\perp}/\Delta_{\perp})^2 \times (L_v/\Delta_v)^2 \times (L_t/\Delta t)$$

# Critical issues for global simulations (I)

## Messo scale transport

- local gyrokinetic turbulence simulations have been found to agree well with experiments in the high temperature core region (r/a<~0.8) of both L-mode and H-mode regimes.
  - Energy fluxes
  - Density fluctuation levels
  - Correlation lengths

- Local gyrokinetic simulations generally under-predict energy transport in the L-mode for r/a>~0.8
- Can the radial propagation of meso-scale non-linear structures explain the systematically under-prediction?  ----> global simulations required

# Critical issues for global simulations (II)
## Turbulence interaction with large scale flows

- Velocity shearing of turbulent fluctuations by large scale flows generate transitions improved confinement regimes. But what is generating the velocity shear?

- $E_r$ radial dependence fairly well predicted by neoclassical theory. However, Reynolds stress from turbulence generate corrugations of Er.
  - Critical for ExB flow shear of the turbulent fluctuations
  - Can transport momentum from the edge to the core

- Coupling of global codes to the edge is essential but extremely challenging: electromagnetic, ions & electrons, geometry, plasma-wall interaction, neutrals.

# Critical issues for global simulations (III)

## Turbulence and MHD modes

- Several global codes have been developed for electromagnetic turbulence to study the self-consistent interplay between magnetic islands and turbulence but are still numerically very challenging.

- The interplay between turbulence and sawtooth/ELM crashes is so far unexplored territory.

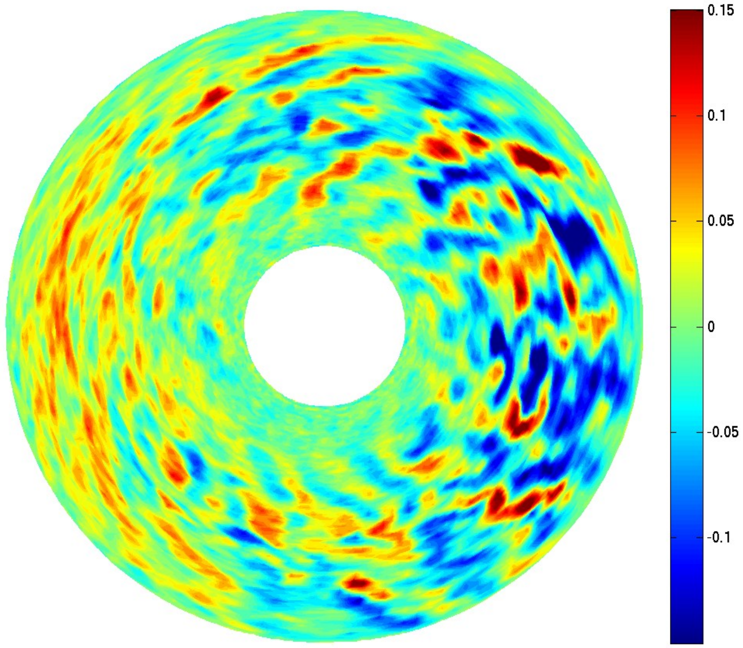
# Numerical PIC approach: ELMFIRE

# Gyrokinetic full-f code: ELMFIRE

## ELMFIRE properties:

- Nonlinear gyrokinetic electrostatic 5D full-f particle code.
- Species: e,i, impurity.
- Binary collision model.
- Quasineutrality enforced through polarization drift and electron parallel non-linearity.
- Applicable for kinetic analysis of neo-classical physics and microturbulence.

Heikkinen et al. JCP '08 & '11, PoP'10




Instantaneous density fluctuation normalized to flux-surface averaged density, poloidal section.

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# Numerical Scheme

$$\frac{dR}{dt} = Ub' + \frac{\mu}{q}\frac{\hat{b} \, x \, \nabla B}{B_\parallel} + \frac{\hat{b} \, x \, \nabla \Phi}{B_\parallel}$$

$$\frac{dv_\parallel}{dt} = \frac{b'}{m}(\mu \nabla B + e \nabla \Phi)$$

Particle initialization on orbits → Particle position → Binary collisions → Displacement of explicit terms → Sampling charge density → Sampling implicit terms in matrix → Solving potential by matrix inversion → Displacement of implicit terms → Data output → Particle position

$$\frac{dR_I}{dt} = \frac{1}{B\Omega}\frac{dE}{dt}$$

$$\frac{dv_{\parallel,e}}{dt} = \frac{qE_\parallel}{2m}$$

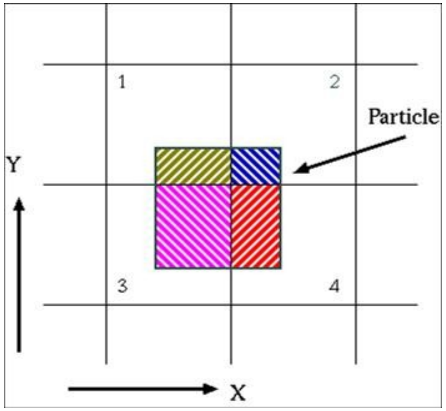

$$\frac{dR_I}{dt} = \frac{1}{B\Omega}\frac{dE}{dt}$$

$$\frac{dv_{\parallel,e}}{dt} = \frac{qE_\parallel}{2m}$$


J.A. Heikkinen PoP 2010

# Momentum or Energy conserving interpolation.

In PIC/CIC scheme one may interpolate in two ways:




1) $E(x)=-\mathrm{grad}\Phi=-\sum\Phi_k \mathrm{grad} S_k(x)$

2) $E(x)=\sum E_k S_k(x)$

Scheme 1) conserves energy and is numerically stable against divergent ExB flow (J.A. Byers et al., 1994) but has a self force.

Scheme 2) conserves momentum, but is prone to numerical instability by divergent ExB flow

# Momentum conserving interpolation scheme drives instabilities by divergent E×B flow

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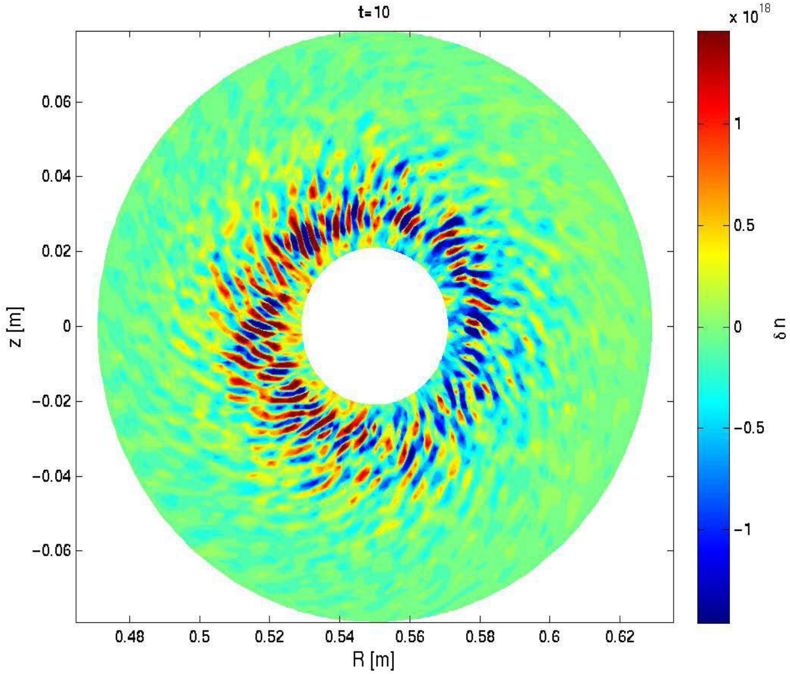



SOLUTION: Ensure zero ExB divergence by modifying the expression for $E_r$.

$$\left(\nabla \times \vec{E}\right)_\phi = 0 \quad \rightarrow \quad \frac{\partial \left(r E_\theta\right)}{\partial r} = \frac{\partial E_r}{\partial \theta}$$

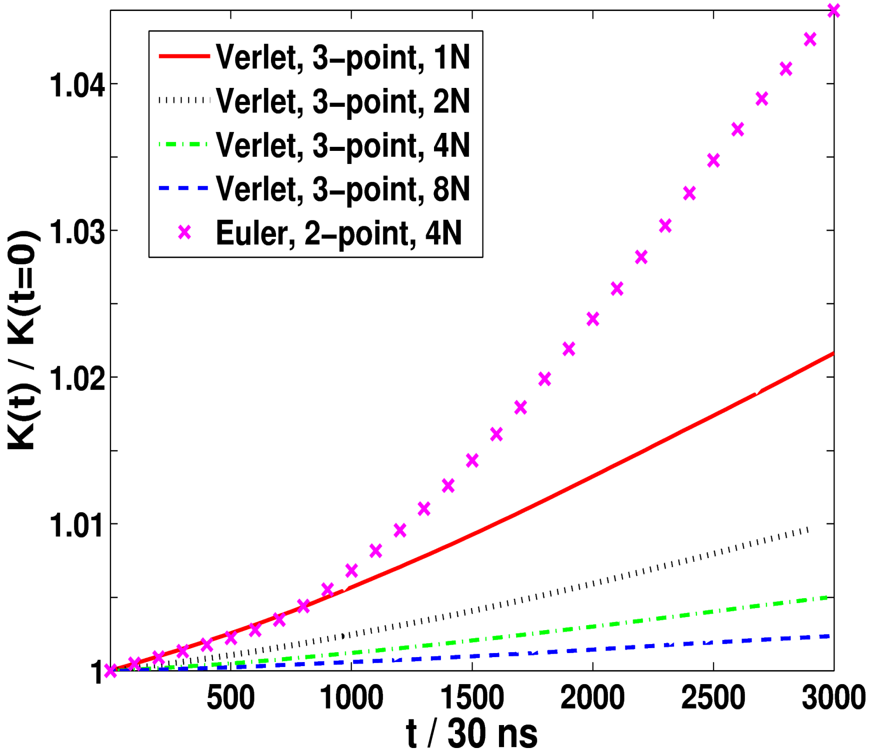
$$E_r(r,\theta,\phi) = \int_0^\theta \frac{\partial}{\partial r}\left(r E_\theta\right) \mathrm{d}\theta + E_r(r,0,\phi)$$

# Energetic consistency

- Where is the energy lost?
  → Electron parallel motion.

- 1st order Implicit Euler tends to cool electrons, only 2-point method stable

- Improvement by using 2nd order velocity verlet integration.



Validation of the ELMFIRE code for ohmic FT-2 tokamak discharges

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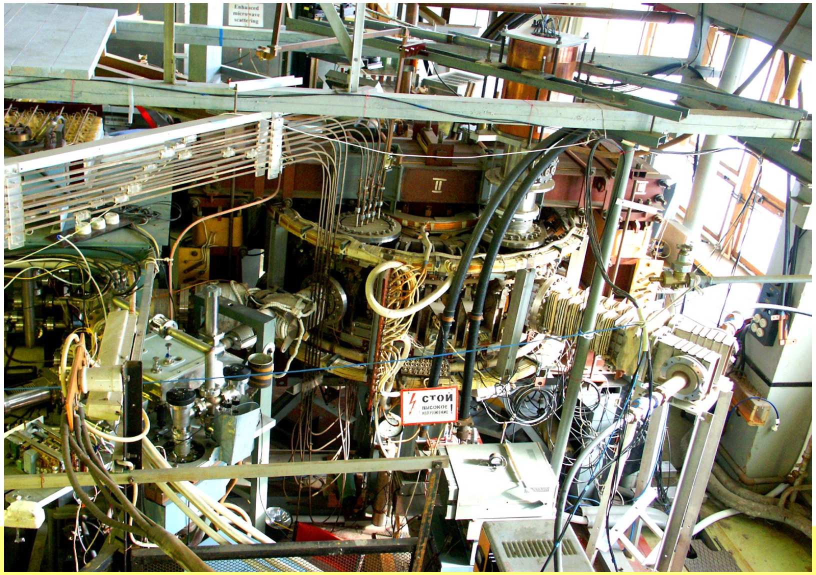
# FT-2 tokamak @ the Ioffe Institute, St. Petersburg

- Large aspect ration: $R_0$ = 55 cm,a = 8 cm

$B_t < 2.7$ T, $I_p < 50$ kA

$N_e < 7 \cdot 10^{19}$ m$^{-3}$, $T_e < 1$ keV, $T_i < 0.4$ keV




- Operational since 1981
- Used for the development of new diagnostics & turbulence and GAM studies

- CX analyser&visible light spectometry
- Multi-pulse Thomson scattering
- Doppler reflectometry: Cutoff layer, $k_\theta \rho_s$~0.1, rad. res. ~0.5 cm
- Enhanced scattering: Upper hybrid resonance layer, $k_\theta \rho_s$~2-5, rad. res. ~0.1 cm

# Confinement time simulation within 5 days with 2048 processors

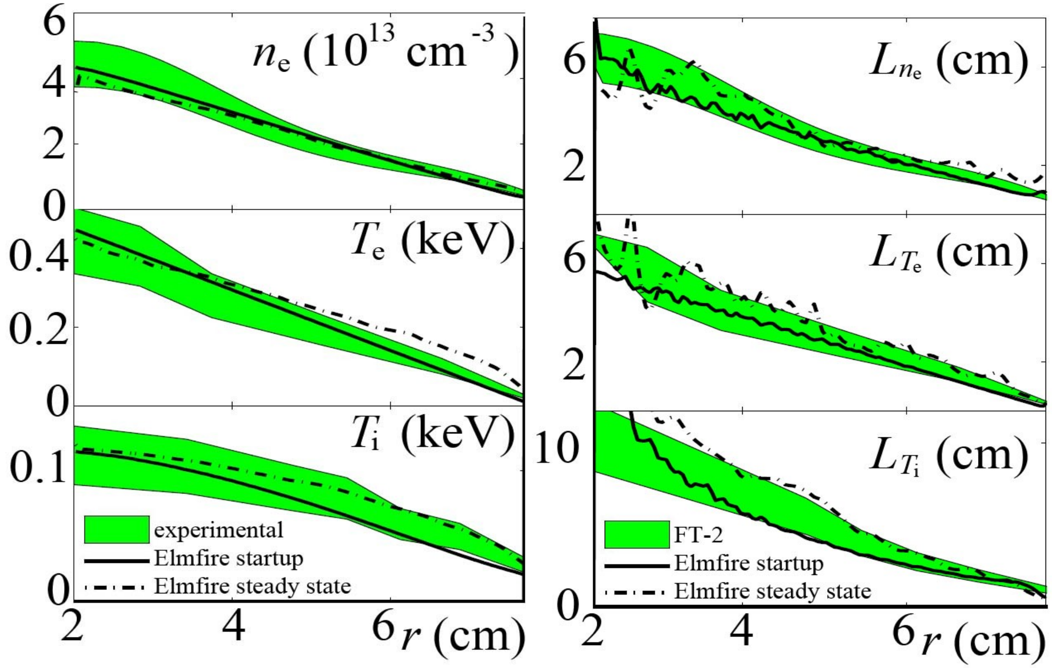
- Confinement time $\tau_E$ ~ 1 ms / 30ns time step ~ 30 000 time steps
- low beta --> electrostatic assumption valid
- large aspect ratio --> analytical magnetic field background

1 time step takes 1 min with 1 000 000 particles per proc.

- High collisionality $\nu^*$ ~ 10-25 & steep gradients ($\delta n/n$~1-8 %)
  - $\rightarrow$ 3000 ppc needed to overcome the noise level
- $1/\rho^* = a/\rho_s = 50\text{-}350$, grid is set to 120r/150p/t8

430 000 000 particles in total

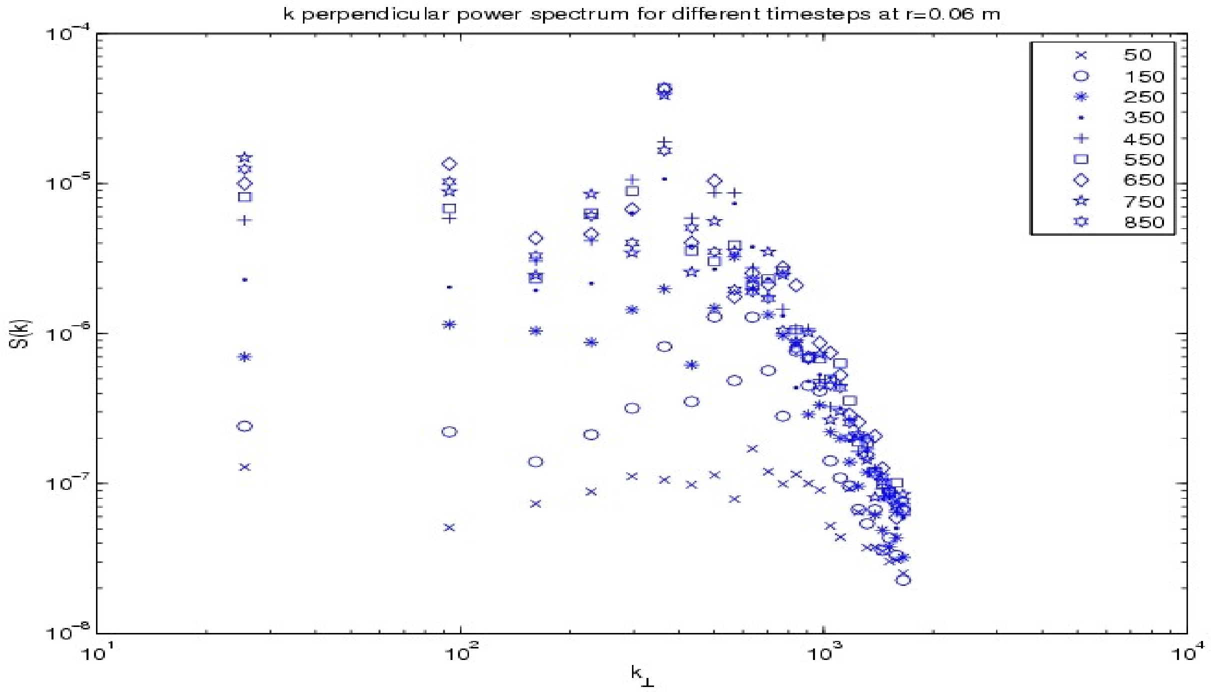
# Steady state profiles obtained 30 µs after start up




B=2.2T, I=18.9 kA,
Hydrogen plasma,
$Z_{eff}$~3.1, Impurity $O^{+6}$

Sources & Sinks
- Ohmic heating model by loop voltage
- radiation & CX losses
- "Poloidal limiter model"
- recycling

# From noise to turbulence spectrum




• Wave number spectrum from different time instants demonstrates how one moves from white noise to physical spectrum in modes.

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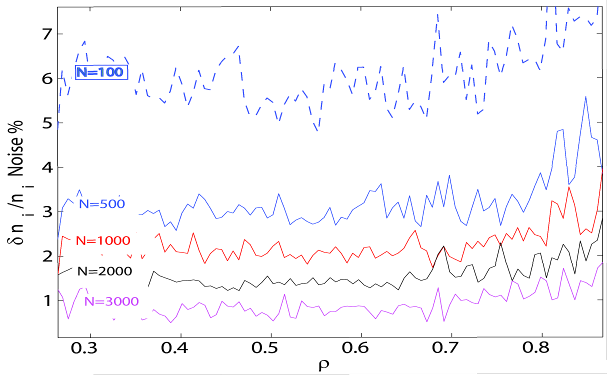
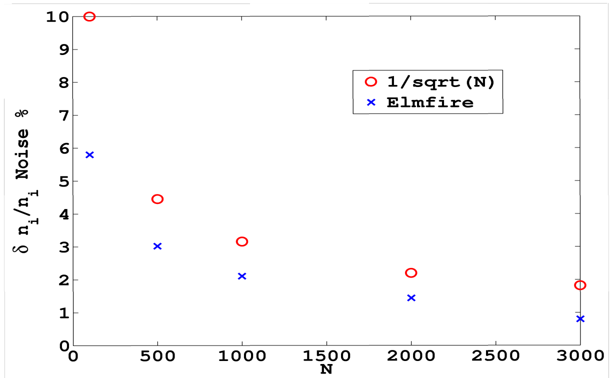
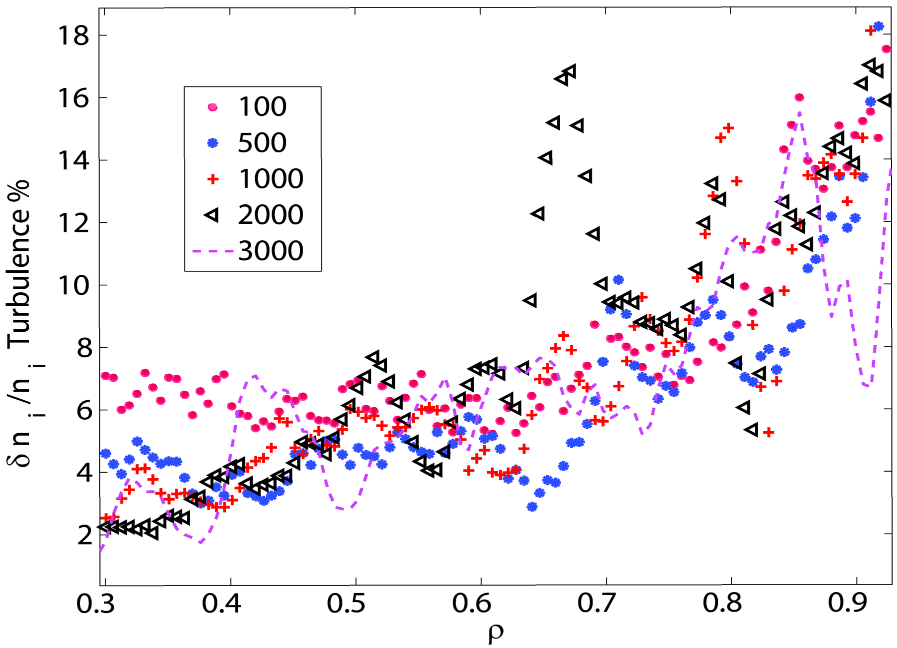
# Noise fluctuation level

Noise level




Turbulence fluctuation level

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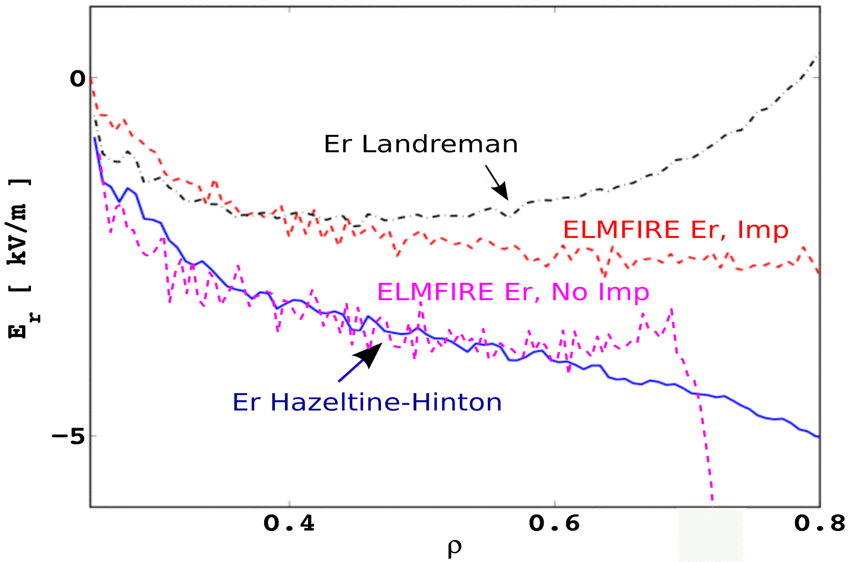
# The Neoclassical equilibrium Er

The neoclassical equilibrium is obtained by removing the modes with toroidal mode number n≠0 => NC filtering




$$E_{r,HH} = \frac{T_i n_i'}{q_i n_i} + C\frac{T_i'}{q_i} + B_p U_i$$

$$C = 1 - \frac{\left(\frac{1.17 - 0.35\sqrt{\nu}}{1 + 0.7\sqrt{\nu}}\right) - 2.1\nu^2 \epsilon^3}{1 + \nu^2 \epsilon^3}$$

The poloidal variation of the impurity density in the presence of steep gradients has an influence on the poloidal flow. Main ions in Plateau regime & Impurities in PS regime

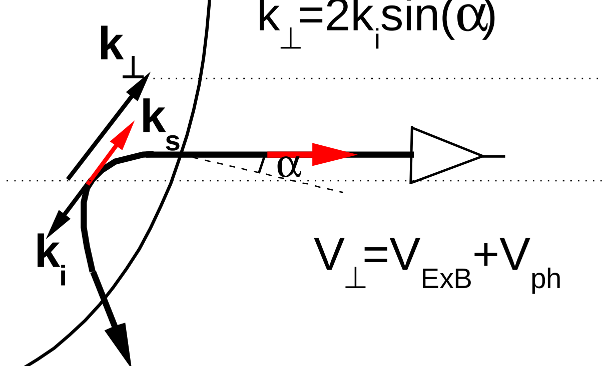
Landreman, PoP 2011

# Synthetic reflectometry diagnostic

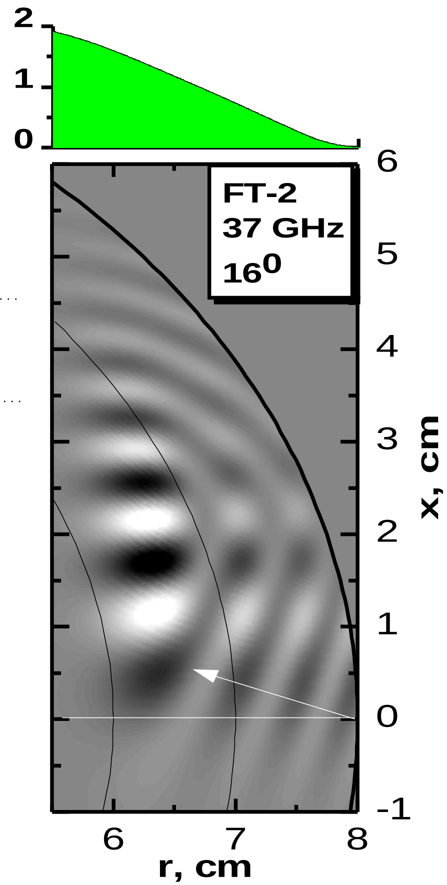
$2\pi\Delta f_D = \mathbf{kV} = k_\perp V_\perp$

$\mathbf{k_\perp = k_s - k_i}$

$k_\perp = 2k_i \sin(\alpha)$




$V_\perp = V_{ExB} + V_{ph}$



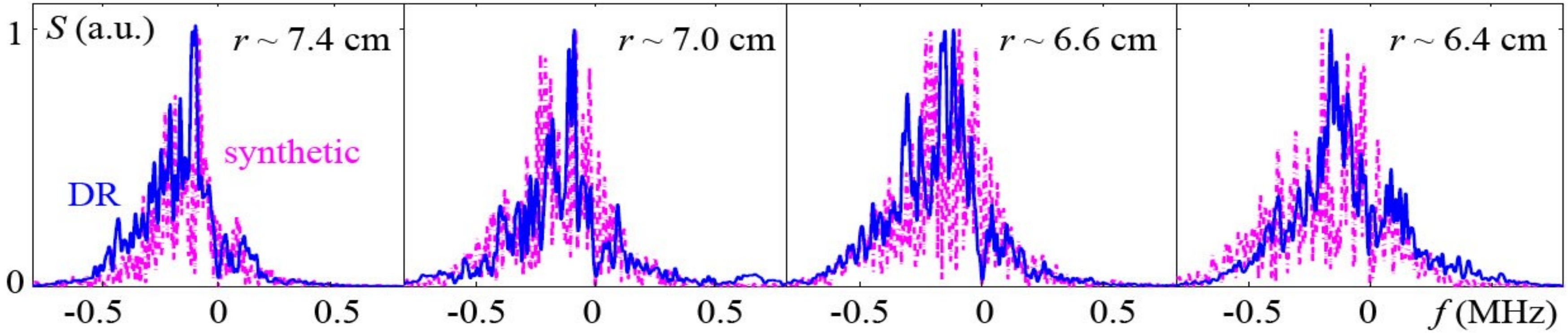

Synthetic diagnostic

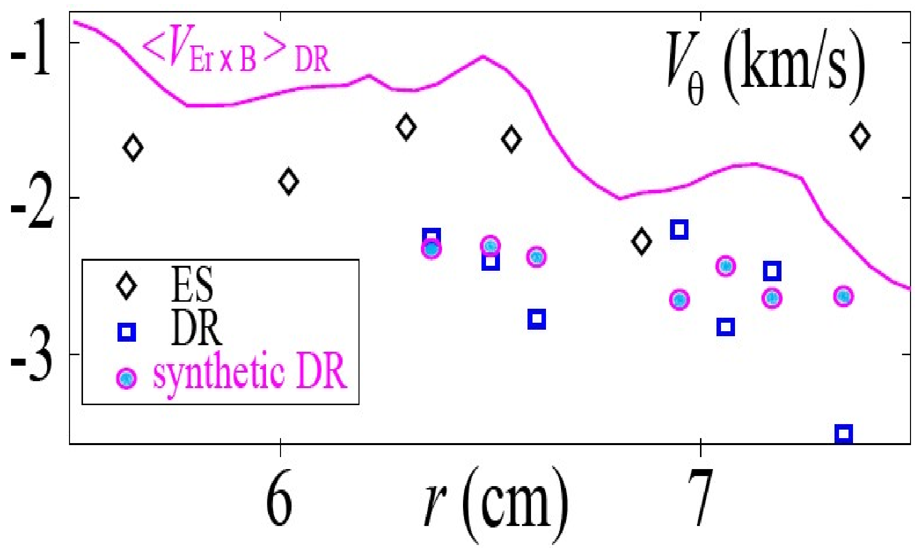
$I(t) = \int w(r,\theta)\, \delta n(r,\theta,t)\, r\, dr\, d\theta$

$W(r,\theta) = w\cos + i^* w\sin$

The synthetic diagnostic is constructed using the complex instrumental DR weighting function.

# Mean poloidal flow is well reproduced by ELMFIRE



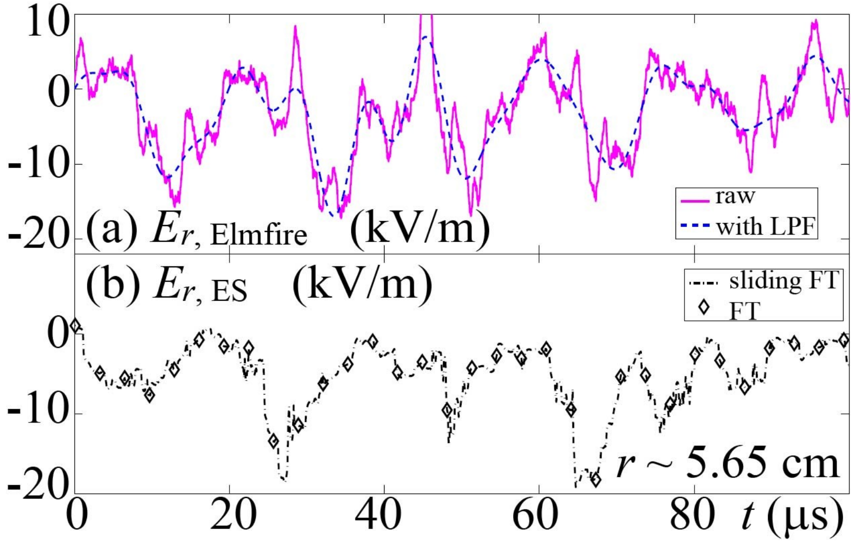



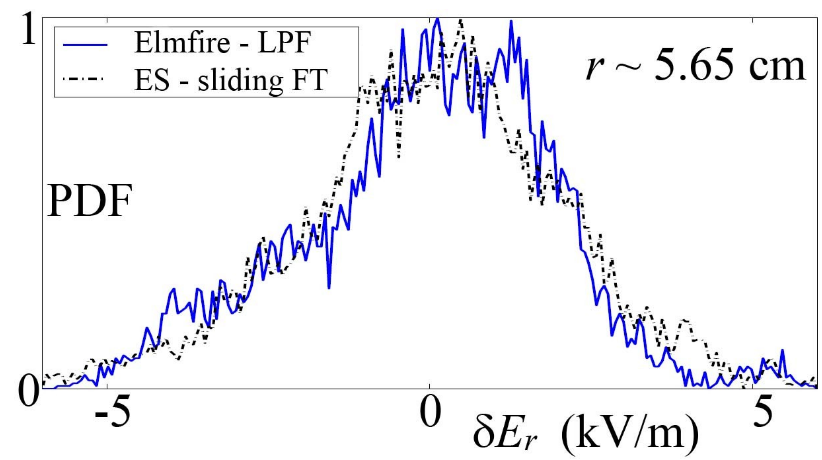

Doppler frequency shift

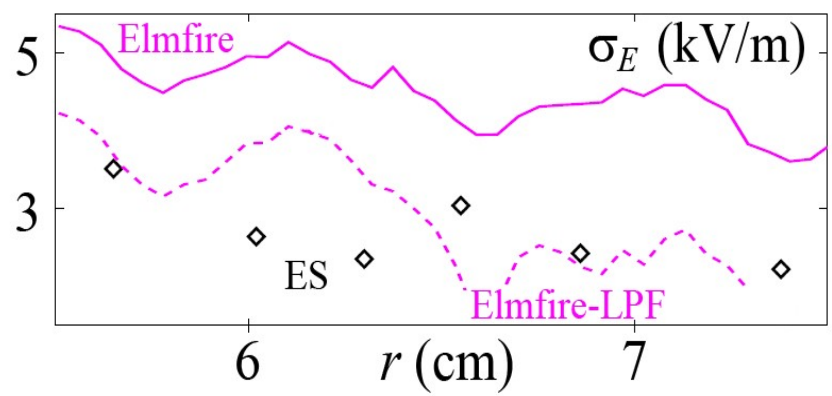
$$f_D = \frac{\int_\Omega f_\Omega |P(f_\Omega)|\, df_\Omega}{\int_\Omega |P(f_\Omega)|\, df_\Omega}$$

$$v_\theta = 2\pi f_D / k_\theta = v_{ExB} + v_{ph}$$

# $E_r$ bursts measured with the ES and reproduced by ELMFIRE



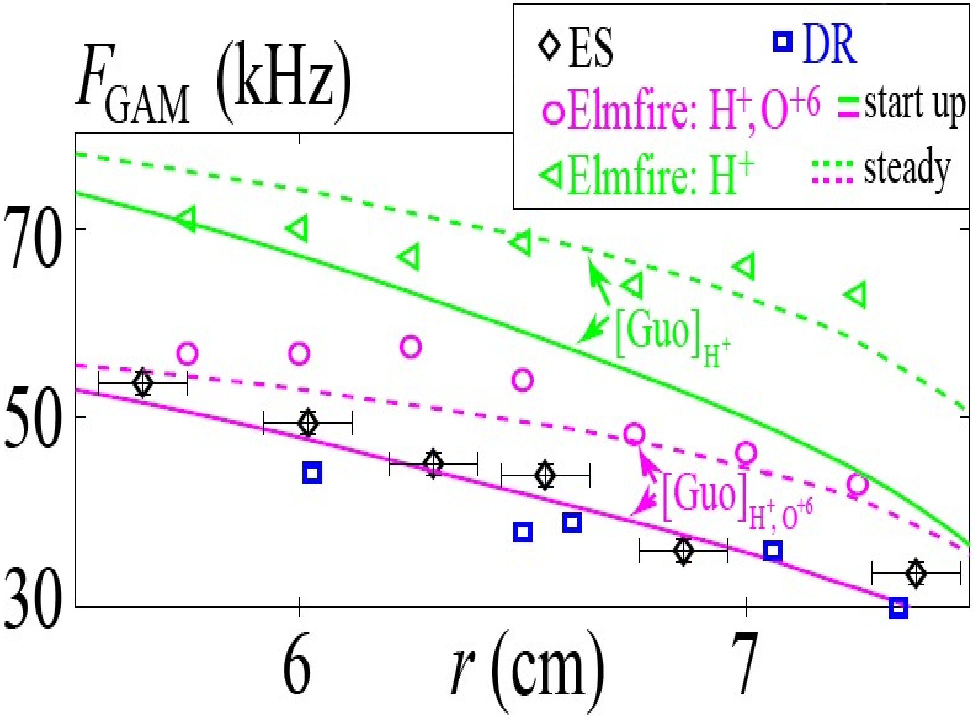




The experimental signal is low-pass filtered with a Nyquist frequency of $F_N$ = 156.25 kHz.

# Effect of the impurities on the GAM frequencies

GAM frequency:

$$\omega_{GAM} = \frac{v_{t,i}}{R}\sqrt{\frac{7}{4} + \frac{T_e}{T_i}}$$




GAM frequency including impurity contribution:

Guo et al. PoP 17 2010

$$\omega_{IMP} = \frac{7/4(n_I + n_Z) + A}{n_I m_I + n_Z m_Z} + \frac{23/8(n_I/m_I + n_Z/m_Z + B)}{7/4(n_I + n_Z) + A} q^2$$

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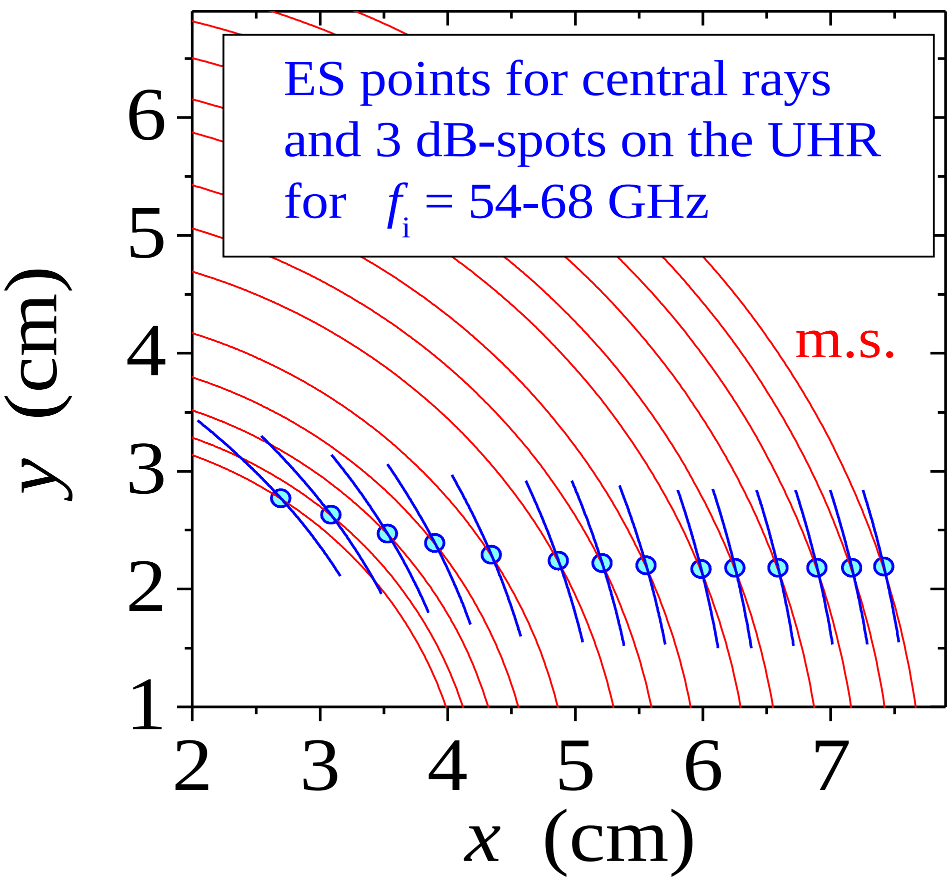
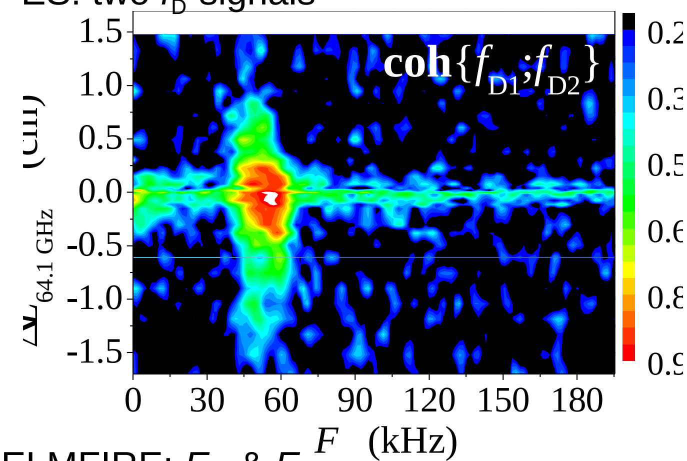
# Correlation measurements with ES Diagnostic



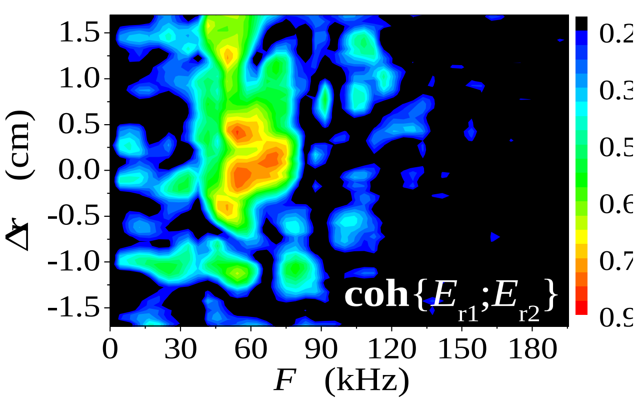

Two signals at probing frequencies with difference $|f_2 - f_1| < 4$ GHz, corresponding to spatial separation $|\Delta L| < 2$ cm in plasma, are measured simultaneously.

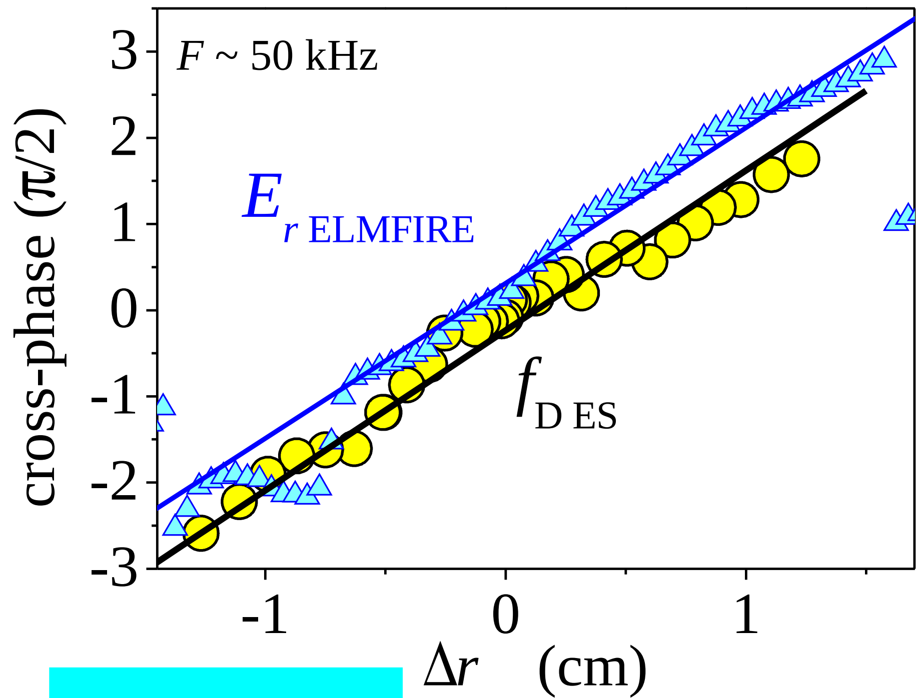
# GAM propagating radially outwards with 1.1 km/s

ES: two $f_D$-signals




ELMFIRE: $E_{r1}$ & $E_{r2}$




$k_r$ ~ 2.8 cm$^{-1}$

$\lambda_r$ ~ 2.2 cm

$V_r$ ~ 1.1 km/s

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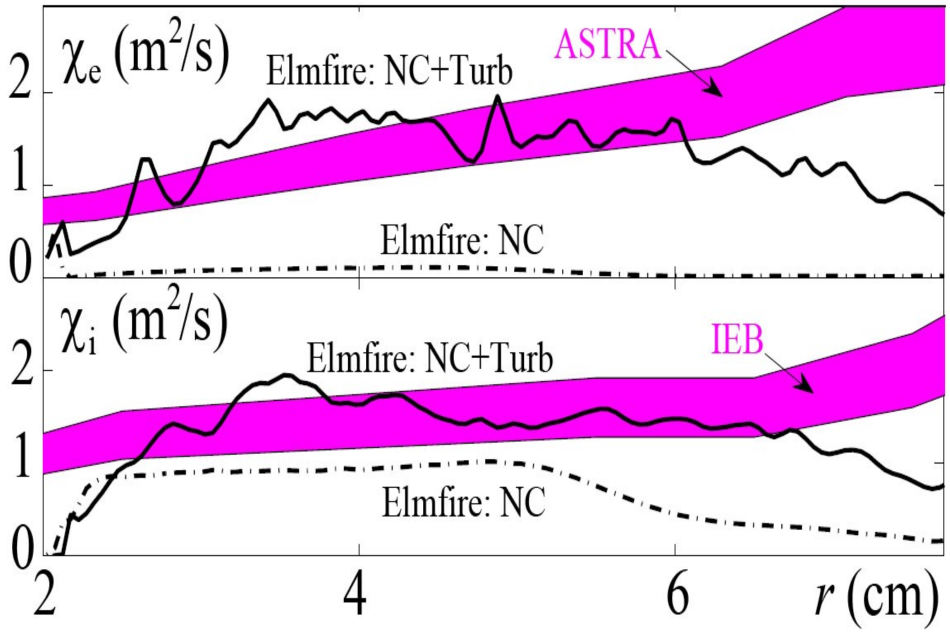
# Profiles and transport results (ctd)




$$\chi_e = \frac{P_{OH} - P_{rad} - \frac{3}{2}\frac{d}{dt}\int n_e T_e \, dV}{4\pi^2 R r n_e \Delta T_e}$$

$$\chi_i = \frac{P_{ei} - P_{CX} - \frac{3}{2}\frac{d}{dt}\int n_i T_i \, dV}{4\pi^2 R r n_i \Delta T_i} h$$

$$\chi = \frac{Q - \frac{3}{2}\Gamma T}{n \Delta T}$$

$$Q = \frac{\sum S(x_p \Delta r)\left(m_p/2\,(v_p - u)^2 - q_p(\Phi_p - \Phi_{FS})\right)}{4\pi^2 R r}$$

<u>What is wrong/missing?</u>

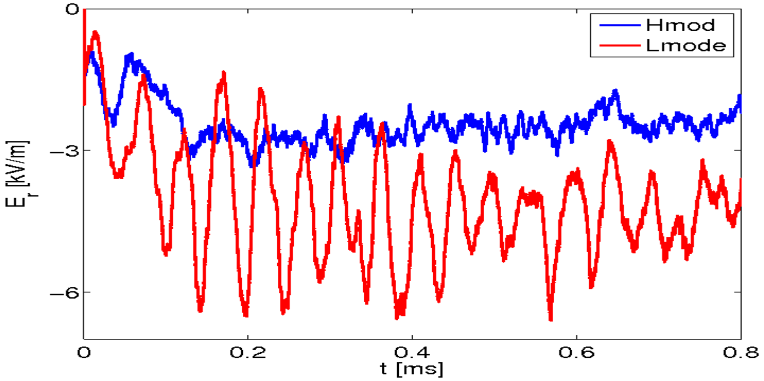
- Definitions of Chi? Grid resolution?
- Boundary treatment? Physics?

# Conclusions

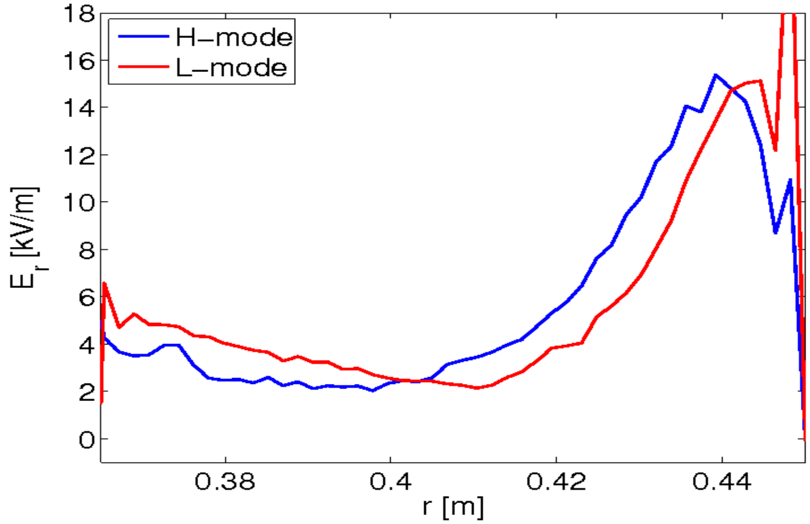
- Good correspondence between experiments and simulation have been obtained for:
  - Mean E×B flows.
  - DR spectra.
  - Oscillations in zonal flows.
  - GAM spatial correlation properties.
- Clear influence of the impurity species on the poloidal flow is observed.
- The transport coefficient agree in size but the trend is opposite.....Why?

# Radial electric field

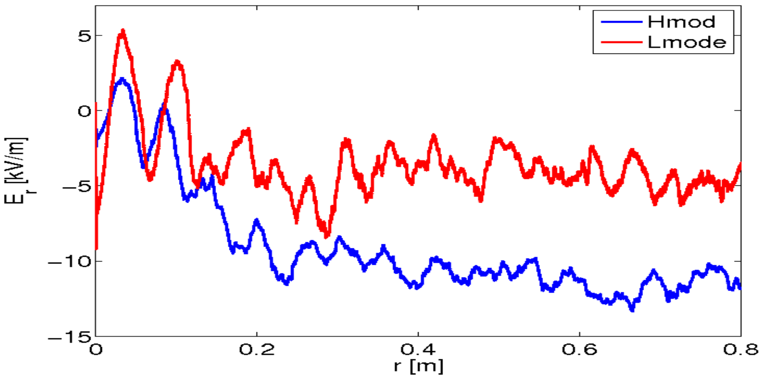
Top pedestal




Radial profile




Half way pedestal

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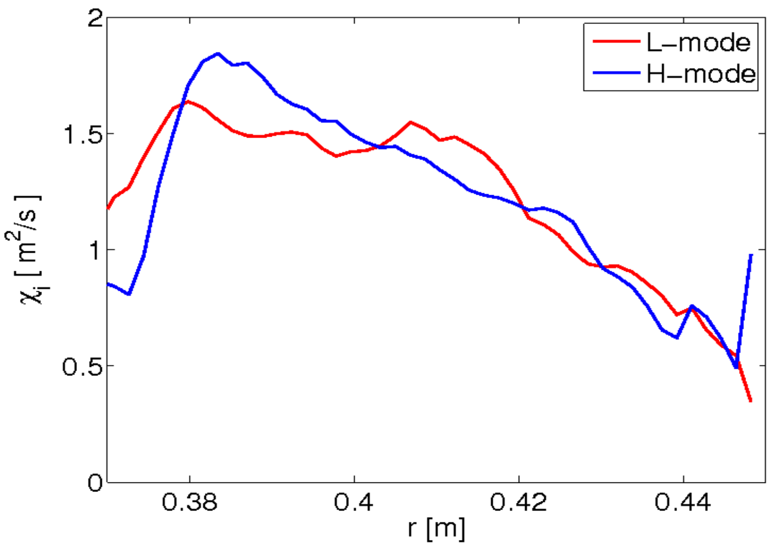
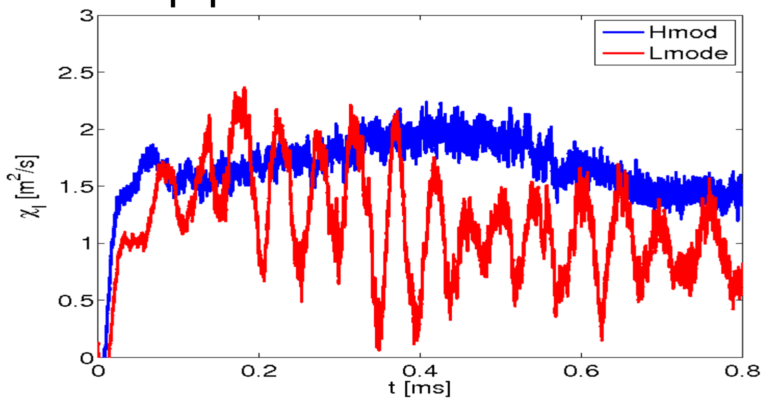
# Ion heat conductivity

Radial profile




Top pedestal

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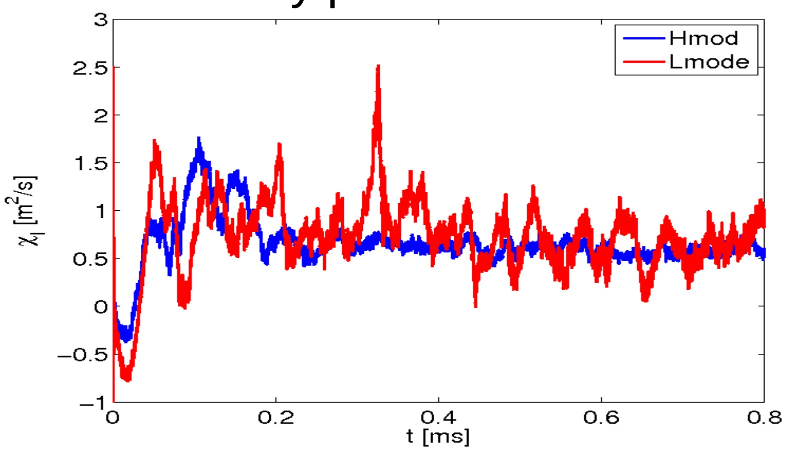
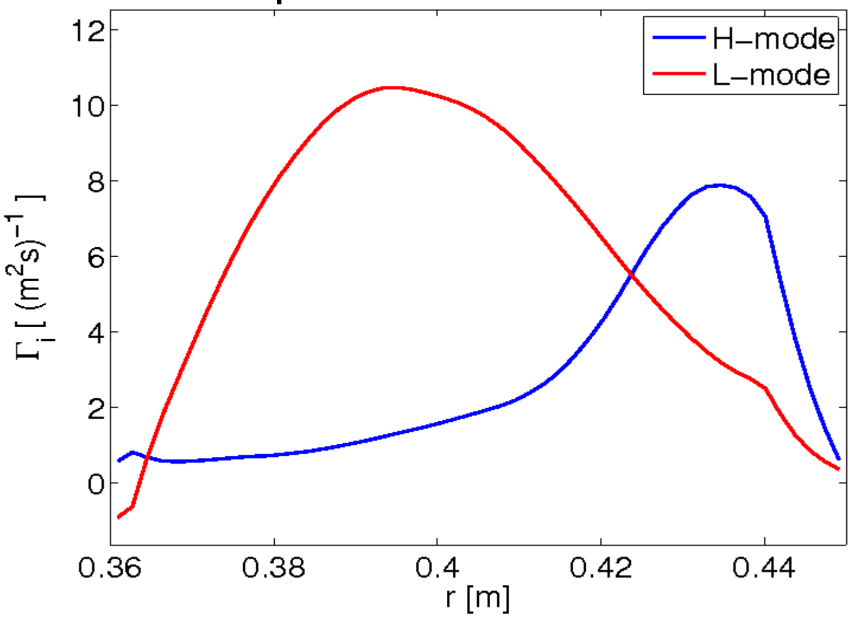
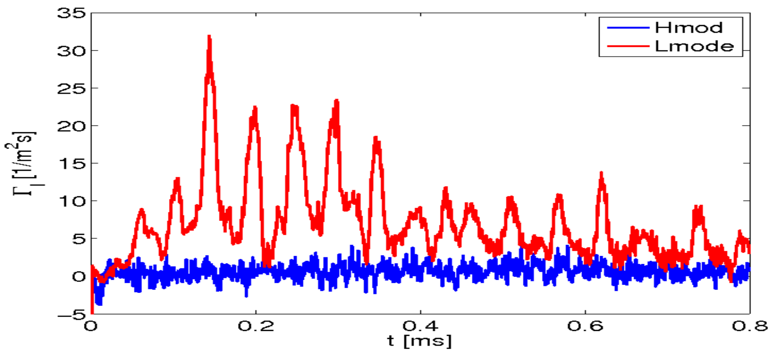


# Ion particle flux

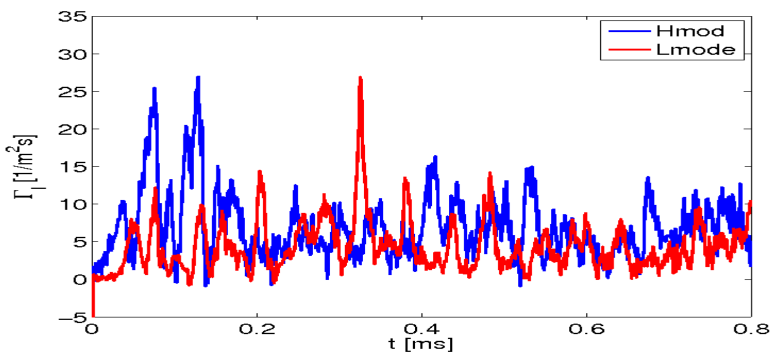
Radial profile




Top pedestal



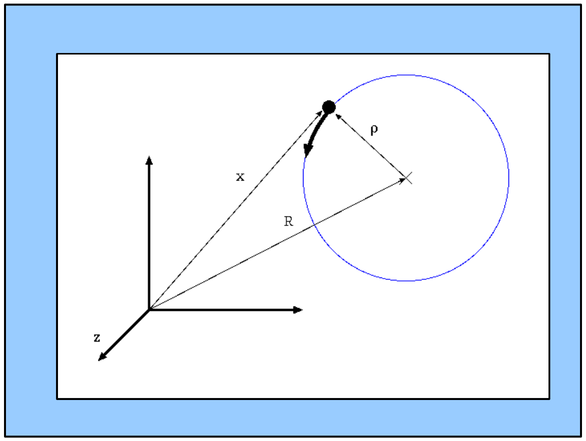

Half way pedestal



# Sosenko's PIC model

- P. Sosenko's model uses an alternative definition of gyrocenter.

  *P.P. Sosenko et al., Physica Scripta 64 (2001) 264*




$$\vec{x} = \vec{R} - \vec{\rho} \qquad \begin{cases} \vec{\rho} = \frac{\vec{b}\times\vec{v}}{\Omega} & \text{Lee} \\ \vec{\rho} = \frac{\vec{b}\times\left(\vec{v}-\vec{V}\right)}{\Omega} & \text{Sosenko} \end{cases}$$

  - Polarization drift is included in the Eqs of motion.
  - This introduces changes on Poisson's equation.

# Sosenko's PIC model

Extra term in the equations of Motion:

$$\frac{dR}{dt} = U\hat{b}_* + \frac{\mu}{e}\frac{\hat{b}\times\nabla B}{B_\parallel} + \frac{\hat{b}\times\nabla\Phi}{B_\parallel} + \frac{1}{\Omega}\frac{d}{dt} - \nabla\Phi$$

$$\frac{dv_\parallel}{dt} = \frac{\hat{b}_*}{m}(\mu\nabla B + e\nabla\Phi)$$

And extra term in the Poisson equation
(for fluid model there is also a Jakobian term in the poisson eq.):

$$\nabla^2\Phi + \frac{q^2}{mBe}\int \left| (\phi - <\phi>)\frac{\delta f}{\delta\mu} + \frac{m}{q} < f > \nabla_\perp^2 < \Phi > \right| dv = \frac{1}{\varepsilon_0}(en_e(\vec{r}) - qn_i(\vec{r}))$$

For $k_\perp\rho_i \to 0, \int |(\Phi - <\Phi>)\frac{\delta f}{\delta\mu} + \frac{m}{q} < f > \nabla_\perp^2 < \Phi > |dv \to 0$