Integrated modelling for fusion devices

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My background

2013	2014- 2019	2019-2021	May 2021- present
Master's- Summer internship at Institute of Plasma Physics (IPR), India	Ph.D. - Theoretical Plasma Physics –Space & astrophysical, Dusty plasmas * **Attended Lindau Nobel Laureates meeting 2016**	ORNL post doc- Started working on energetic particle physics in fusion plasmas	ORNL staff position- *Theory and Computation Plasma physicist*

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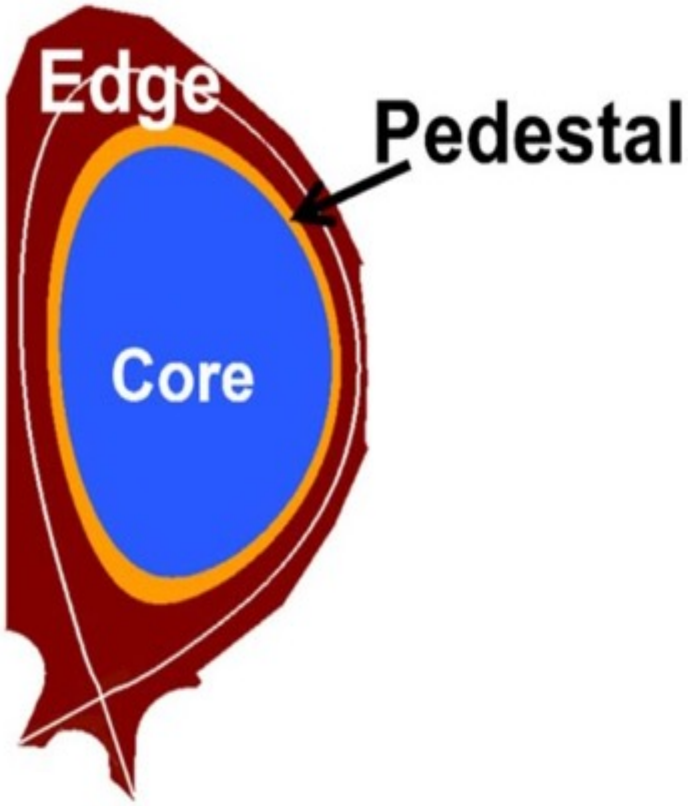
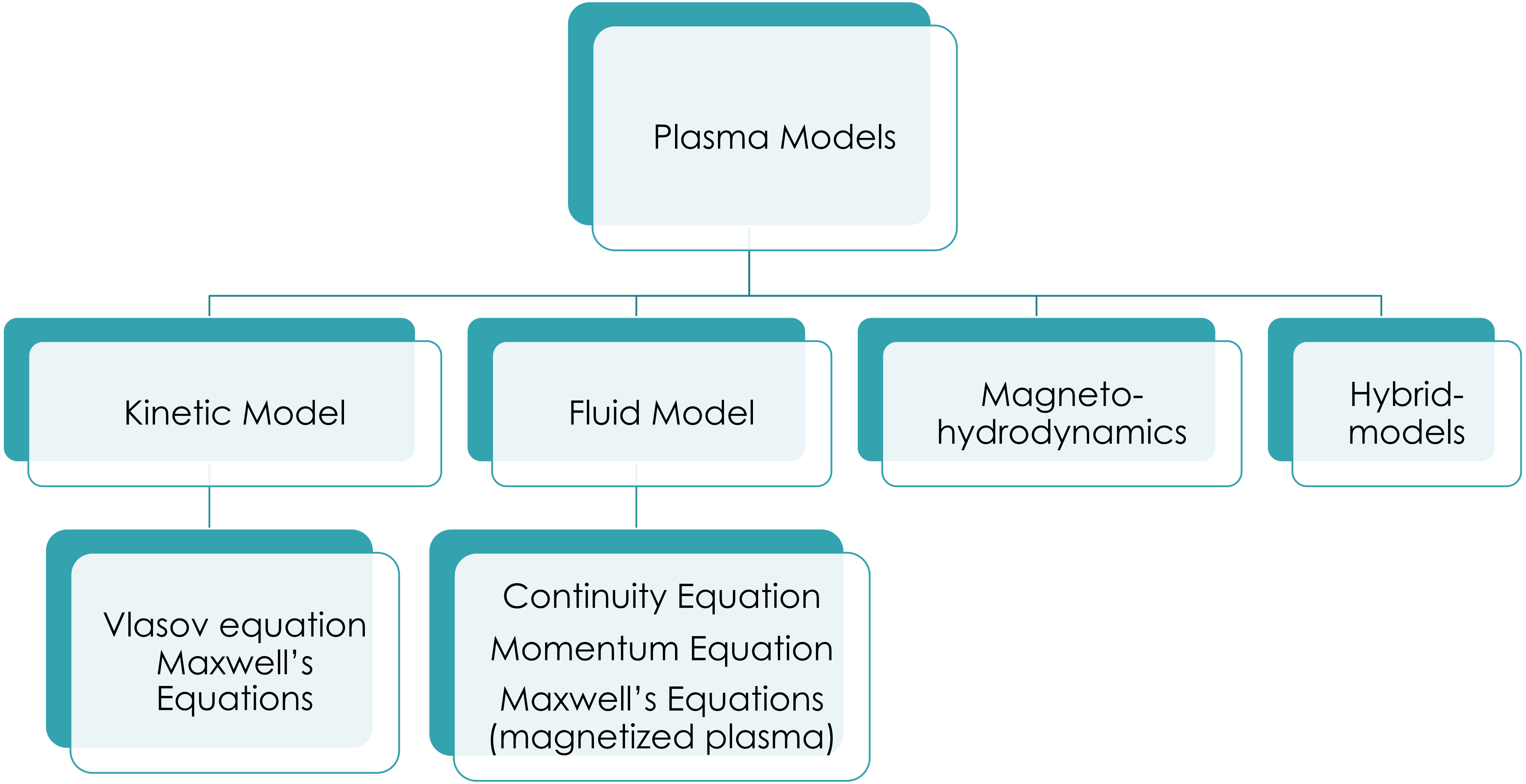
Key Takeaways

- Different theoretical and numerical models are used to describe the distinct plasma properties in the core and edge regions.
- **Integrated modelling is needed to perform comprehensive simulations of various physical processes and interactions within a fusion reactor**
- Combination of multiple models to optimize performance and predict behavior of a future reactor-relevant fusion device.



Theoretical descriptions of Plasma



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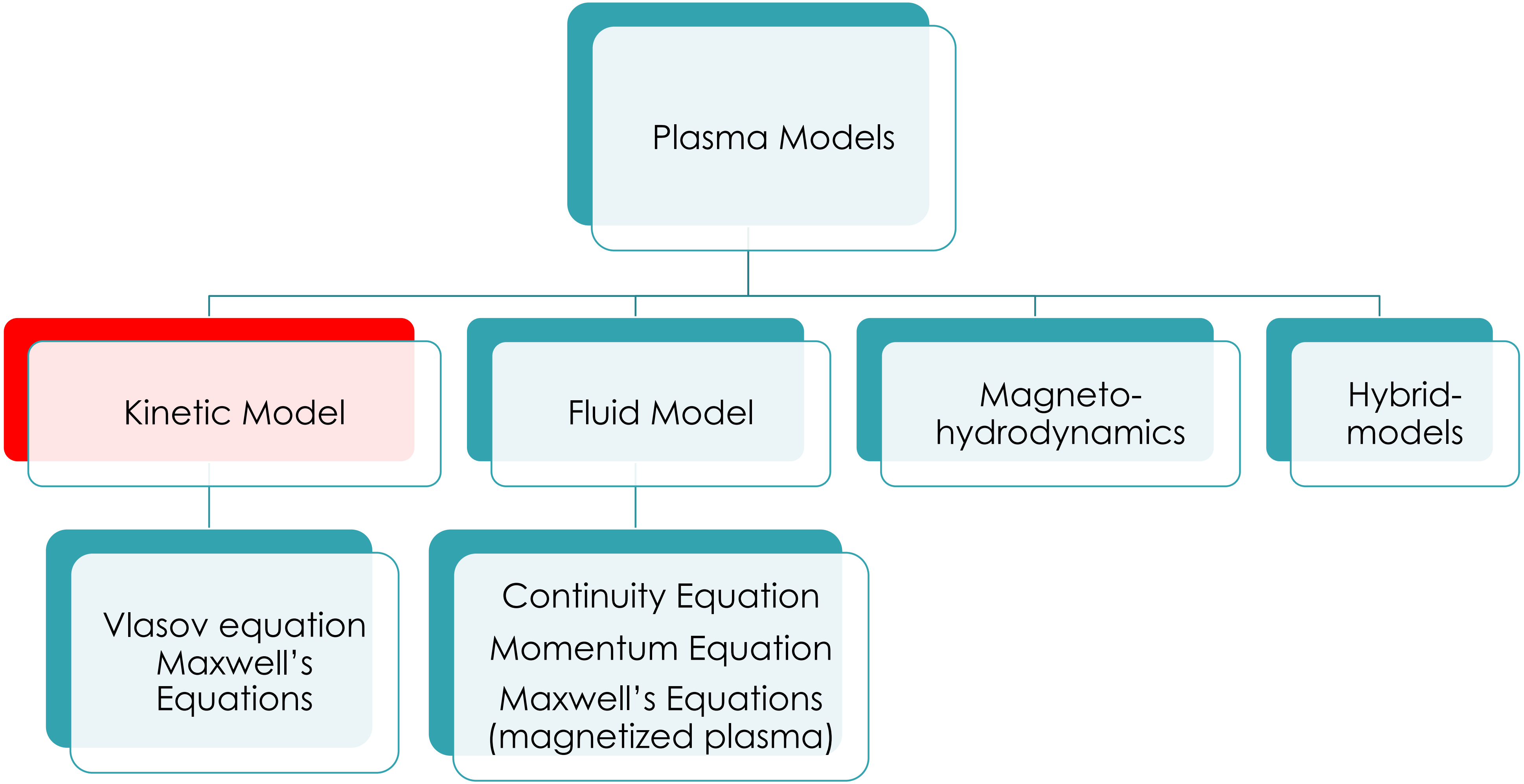


Kinetic description

Assumption: on average, behavior of each particle is the same and independent of other particles, following only the prescriptions of the self-consistent field – collisionless plasma

Boltzmann equation

$$\frac{\partial f}{\partial t} + \vec{v}\frac{\partial f}{\partial \vec{r}} + \dot{\vec{v}}\frac{\partial f}{\partial \vec{v}} = \left(\frac{df}{dt}\right)_{\text{coll}}$$

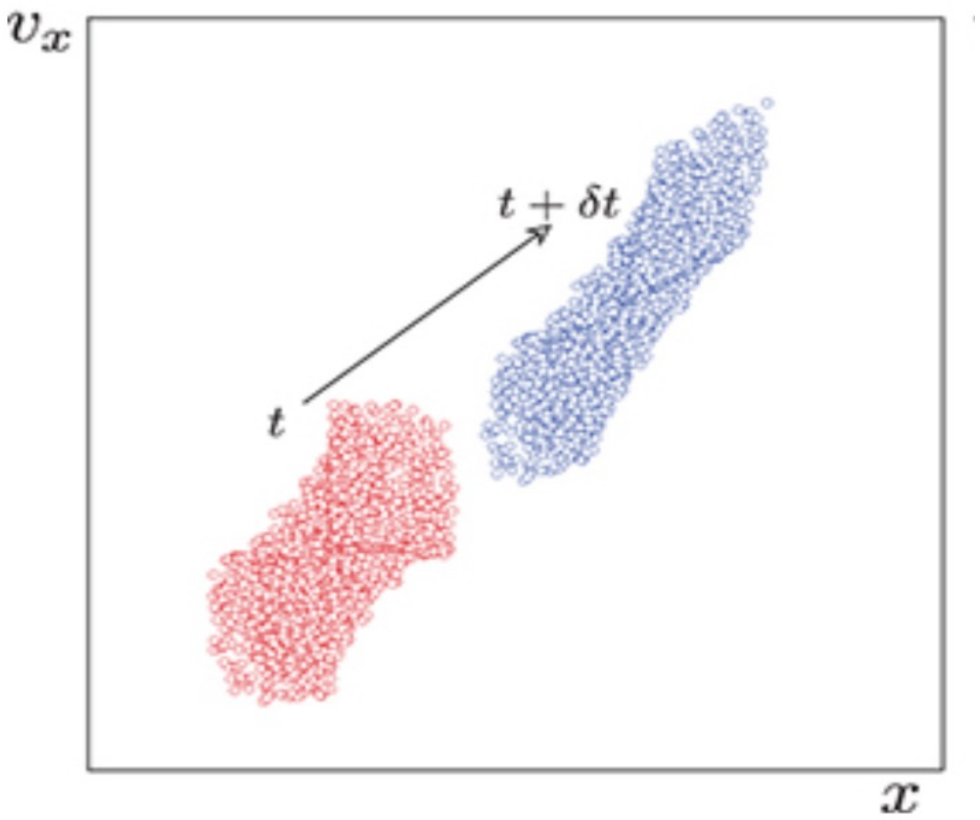
Kinetic Vlasov-equation

$$\frac{\partial f}{\partial t} + \vec{v}\nabla f + \frac{e}{m}(\vec{E} + \frac{1}{c}[\vec{v} \times \vec{B}])\frac{\partial f}{\partial \vec{v}} = 0$$

Maxwell's equations

$$\nabla \times \vec{E} = -\frac{1}{c}\frac{\partial B}{\partial t} \qquad \nabla \vec{B} = 0$$

$$\nabla \times \vec{B} = \frac{1}{c}\frac{\partial \vec{E}}{\partial t} + \frac{4\pi}{c}\vec{j} \qquad \nabla \vec{E} = 4\pi q,$$



Description of plasma in 2-D phase-space

$$f = f(\vec{r}, \vec{v}, t)$$

is the charged particle distribution function in 6-D position momentum space

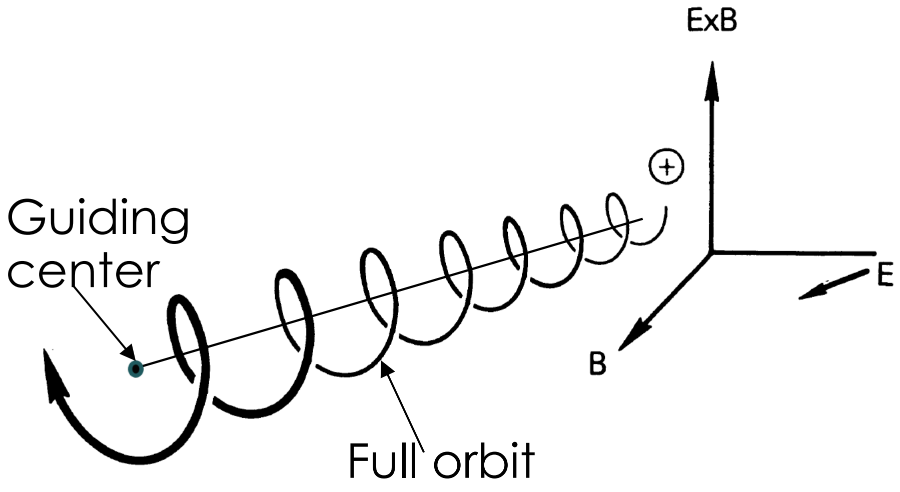
Due to strong magnetic fields in fusion plasmas, we take average of the Vlasov equation over the fast gyromotion, which leads to gyrokinetic equation

Gyrokinetic equation in fusion plasmas

$$\frac{\partial h_s}{\partial t} + \left(v_{||}\hat{b} + \vec{V}_{ds} + \left\langle \vec{V}_\phi \right\rangle_\varphi \right) \cdot \vec{\nabla}_{\vec{R}} h_s - \sum_{s'} \left\langle C\left[h_s, h_{s'}\right] \right\rangle_\varphi = \frac{Z_s e f_{s0}}{T_s} \frac{\partial \langle \phi \rangle_\varphi}{\partial t} - \frac{\partial f_{s0}}{\partial \psi} \left\langle \vec{V}_\phi \right\rangle_\varphi \cdot \vec{\nabla}\psi.$$

Perturbed distribution function

$$h_s \equiv f_{s1} + \frac{Z_s e \phi}{T_s} f_{s0}$$



+ Gyro-averaged Maxwell's equation (Electromagnetic waves) / Gauss's law (Electrostatic waves)

Theoretical descriptions of Plasma

- Plasma Models
  - Kinetic Model
    - Vlasov equation
      Maxwell's Equations
  - Fluid Model
    - Continuity Equation
      Momentum Equation
      Maxwell's Equations (magnetized plasma)
  - Magneto-hydrodynamics
  - Hybrid-models

When we take moments of kinetic-Vlasov equation, we obtain fluid equations for plasma

Average behavior of each species is sufficient to describe plasma dynamics- collisional plasmas

Zeroth order moment : fluid density “n”
$n = \iiint_{-\infty}^{\infty} f \; d^3v$

$$\frac{\partial}{\partial t} n + \nabla . (n \, u) = 0$$

First order moment : Fluid velocity “u”
$\mathrm{n}\, u = \iiint_{-\infty}^{\infty} vf \; d^3v)$:

$$nm \left[\frac{\partial u}{\partial t} + (u \; \cdot \nabla) u \right] = nq[E + u \times B] - \nabla p$$

+ Maxwell’s equation (Electromagnetic waves) / Gauss’s law (Electrostatic waves)

Moments of gyrokinetic equation lead to gyrofluid equations for strongly magnetized plasma

Zeroth order: $\frac{\partial n_f}{\partial t} = -v_{\zeta,eq}\frac{\partial n_f}{\partial \zeta} - \frac{{v_{th,f}}^2}{\epsilon^2 \Omega_{c,f}}\left(\Omega_d\left(n_f\right)\right) - n_{0,f}\nabla_\parallel u_{\parallel,f} - n_{0,f}\ \Omega_d(\phi) + n_{0,f}$ $\Omega_*(\phi)$

First order : $\frac{\partial u_{\parallel,f}}{\partial t} = -v_{\zeta,eq}\frac{\partial u_{\parallel,f}}{\partial \zeta} - \frac{4{v_{th,f}}^2}{\epsilon^2 \Omega_{c,f}}\ \Omega_d(u_\parallel) - \left(\frac{\pi}{2}\right)^{\frac{1}{2}} v_{th,f}\left|\nabla_\parallel\left(v_{\parallel,f}\right)\right| - \frac{{v_{th,f}}^2}{n_{0,f}}\nabla_\parallel\left(n_f\right)$

$+{v_{th,f}}^2(1+\eta)\Omega_*(\psi) + v_{th,f}\ \ \Omega_*(\phi)$

Closure coefficient

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Fluid model in a magnetized plasma can be simplified to MHD model

2-Fluid model

$$\frac{\partial n_e}{\partial t} + \nabla \cdot (n_e \mathbf{u}_e) = 0,$$

$$\frac{\partial n_i}{\partial t} + \nabla \cdot (n_i \mathbf{u}_i) = 0,$$

$$0 = -en_e(\mathbf{E} + \mathbf{u}_e \times \mathbf{B}) - \nabla p_e - m_e n_e \overline{\nu}_{ei}(\mathbf{u}_e - \mathbf{u}_i),$$

$$m_i n_i \left(\frac{\partial}{\partial t} + \mathbf{u}_i \cdot \nabla\right) \mathbf{u}_i = en_i (\mathbf{E} + \mathbf{u}_i \times \mathbf{B}) - \nabla p_i - m_e n_e \overline{\nu}_{ei} (\mathbf{u}_i - \mathbf{u}_e),$$

$$\frac{3}{2} n_e \left(\frac{\partial}{\partial t} + \mathbf{u}_e \cdot \nabla\right) T_e + p_e \nabla \cdot \mathbf{u}_e + \nabla \cdot \mathbf{q}_e = S_e,$$

$$\frac{3}{2} n_i \left(\frac{\partial}{\partial t} + \mathbf{u}_i \cdot \nabla\right) T_i + p_i \nabla \cdot \mathbf{u}_i + \nabla \cdot \mathbf{q}_i = S_i,$$

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t},$$

$$\nabla \times \mathbf{B} = \mu_0 e(n_i \mathbf{u}_i - n_e \mathbf{u}_e),$$

$$n_i - n_e = 0,$$

$$\nabla \cdot \mathbf{B} = 0.$$

Single fluid Magnetohydrodynamic model

mass : $\frac{d\rho}{dt} + \rho \nabla \cdot \mathbf{v} = 0;$

momentum : $\rho \frac{d\mathbf{v}}{dt} = \mathbf{J} \times \mathbf{B} - \nabla p;$

Ohm's law : $\mathbf{E} + \mathbf{v} \times \mathbf{B} = 0$ ideal MHD,

$\mathbf{E} + \mathbf{v} \times \mathbf{B} = \eta_{\parallel} \mathbf{J}$ resistive MHD;

energy : $\frac{d}{dt}\left(\frac{p}{\rho^{\gamma}}\right) = 0;$

Maxwell : $\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t},$

$\nabla \times \mathbf{B} = \mu_0 \mathbf{J},$

$\nabla \cdot \mathbf{B} = 0.$

Where, $\rho = \frac{m_i n_i + m_e n_e}{m_i + m_e} \equiv m_i n;$ $\rho = \frac{m_i n_i u_i + m_e n_e u_e}{m_i n_i + m_e n_e} \equiv u_i;$ $J = en(u_i - u_e)$

$p \equiv p_e + p_i$

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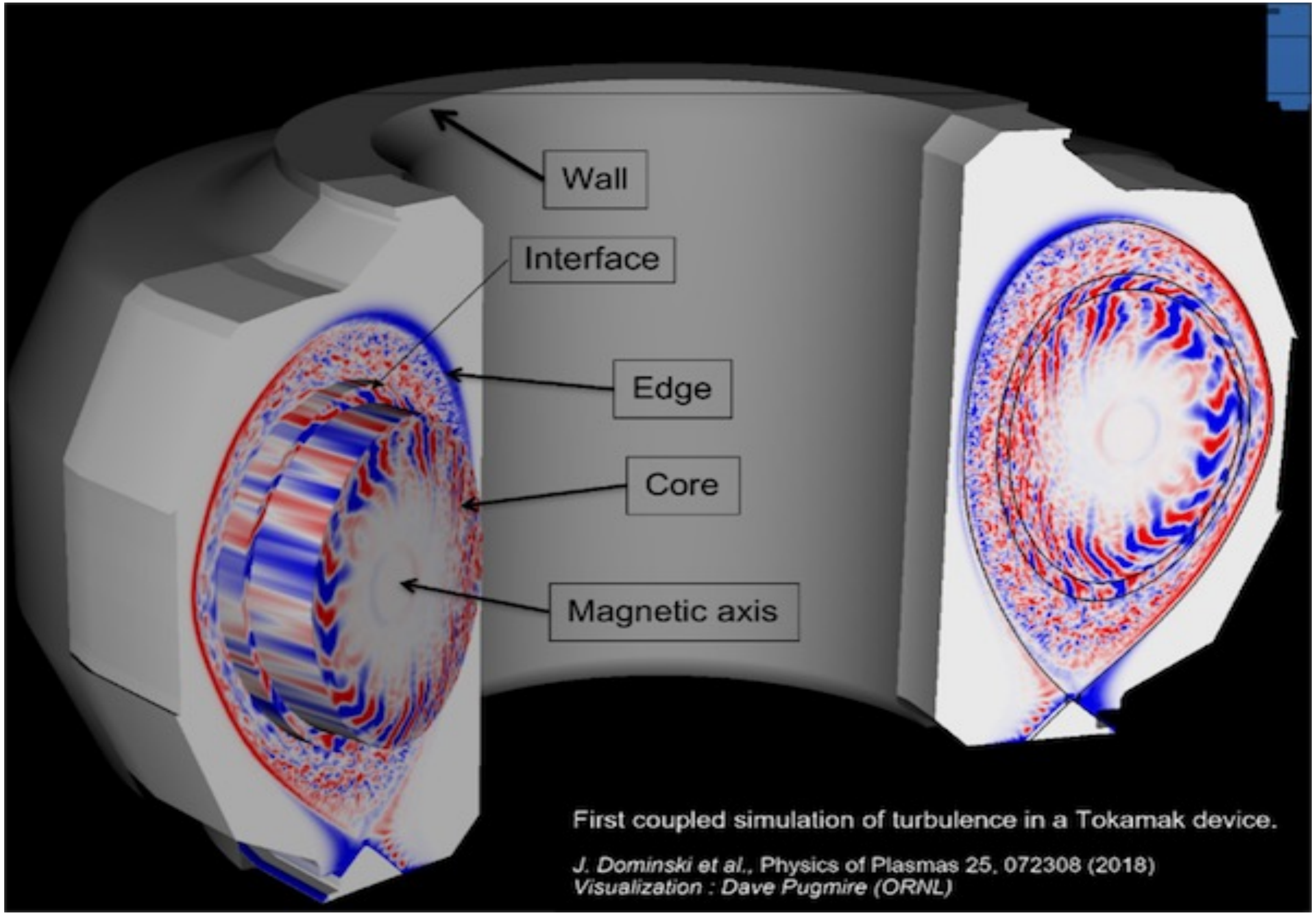
Plasma modelling is to solve the differential equations and identify the spatiotemporal behavior of a plasma system

- Depending upon the physics we want to resolve, we simplify our models by making assumptions
- Discretize equations and use numerical techniques such as finite difference, finite elements for fluid equations
- Runge-Kutta integrators for particle orbit following codes
- PIC approach for solving kinetic equations
- Finite difference, finite element/volume scheme for solving fluid equations

Core and edge plasma conditions are very different in a fusion device

Property	Fusion Plasma Core	Fusion Plasma edge
Temperature	Extremely high, ~keV	Much cooler compared to the core (1-100 eV)
Density	Higher particle density	Lower particle density
Magnetic fields	Stronger and more uniform	Weaker and more turbulent
Particle behavior	Highly energized and relatively stable	More turbulent and irregular
Confinement	Better confinement properties	Poorer confinement due to increased turbulence
Impurities	Relatively cleaner with fewer impurities	More impurities from interactions with reactor walls

Dynamics of core plasmas are defined by gyrokinetic models whereas edge plasmas are defined by fluid models

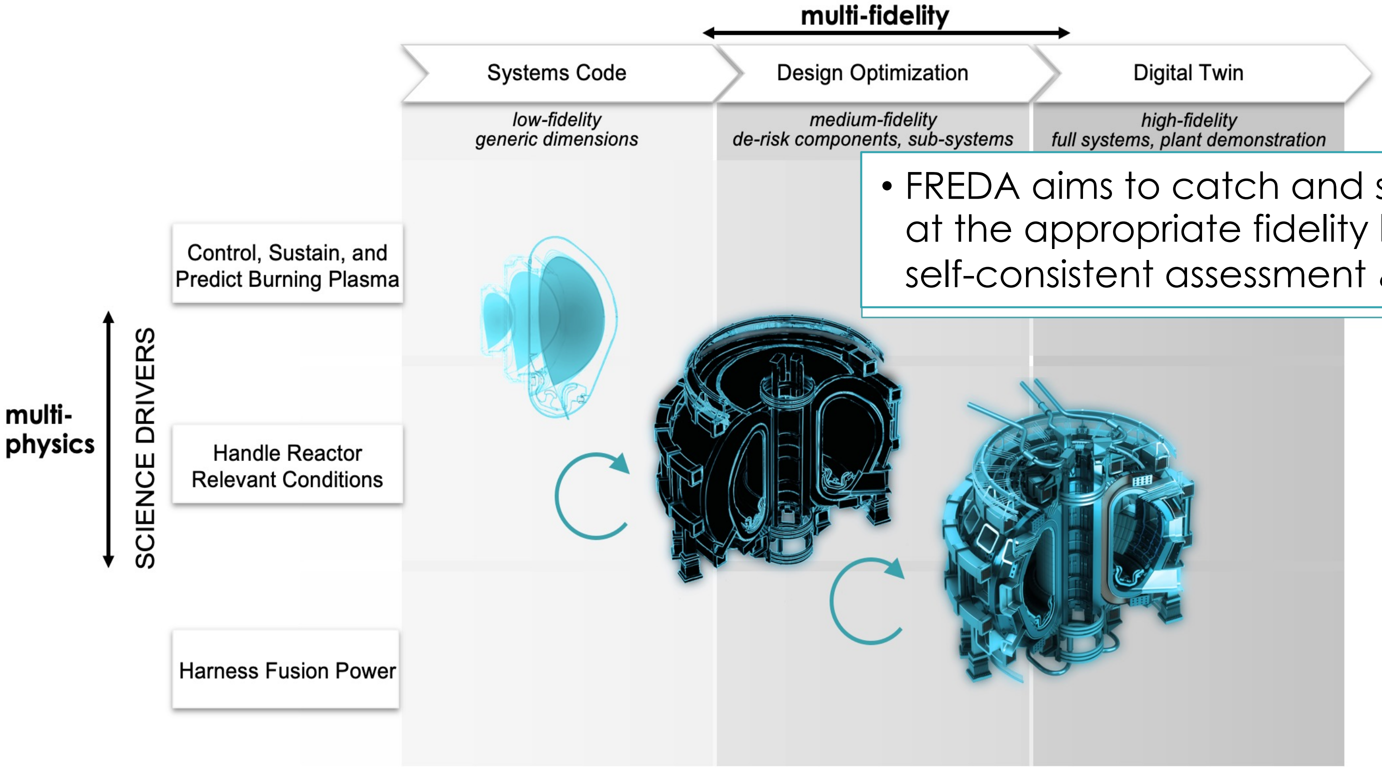


Integrated Modelling for fusion reactor design

What is integrated modeling?

Coupled models of fusion plasma physics and engineering in an integrated workflow to perform self-consistent multi-physics, multi-fidelity, iterative calculations for a fusion reactor design

FREDA (Fusion Reactor Design and Assessment)-SciDAC is a purpose-built framework for multi-fidelity, iterative optimization- led by Cami Collins, ORNL



- FREDA aims to catch and solve 'show-stoppers' at the appropriate fidelity level using self-consistent assessment & design optimization

Will initially apply to tokamaks/STs, potential for expansion to stellarators

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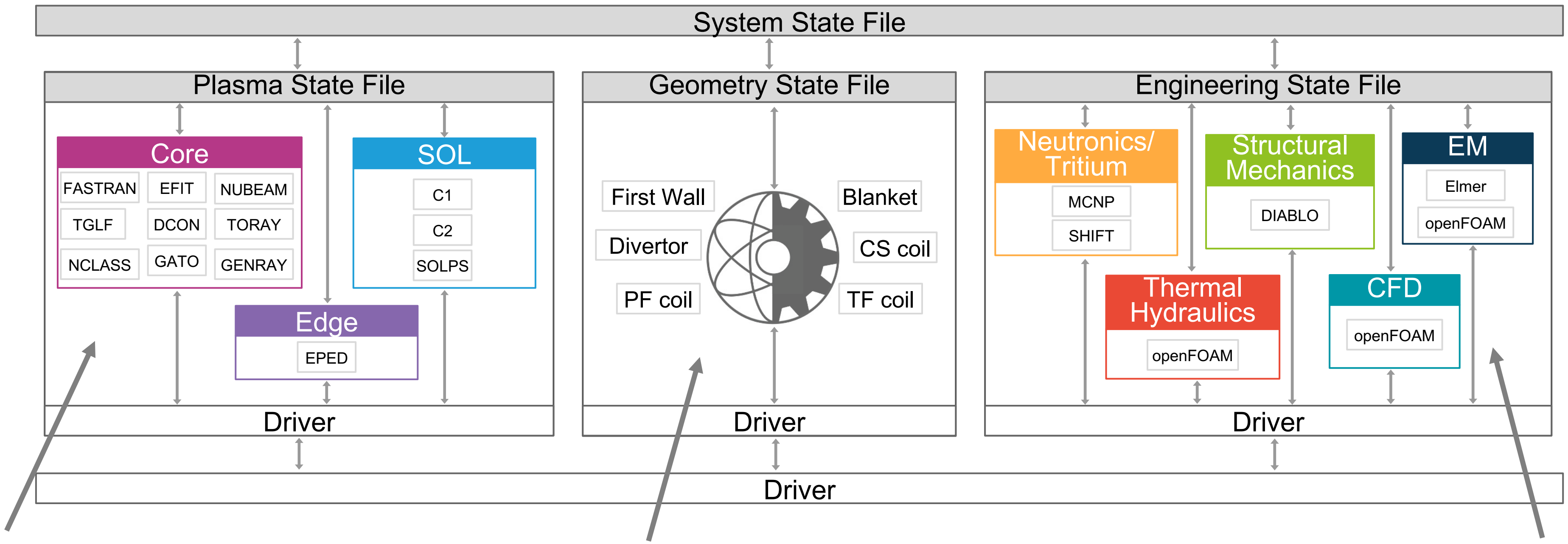
Approach: flexible component-based framework & data structure

Framework & Workflow

Capable of integrating swappable modules with diverse CPU/GPU requirements



Fusion-Plasma

- Based on the open-source IPS (Integrated Plasma Simulator)

Parametric Geometry

- Includes systems codes and parameterized geometry representation

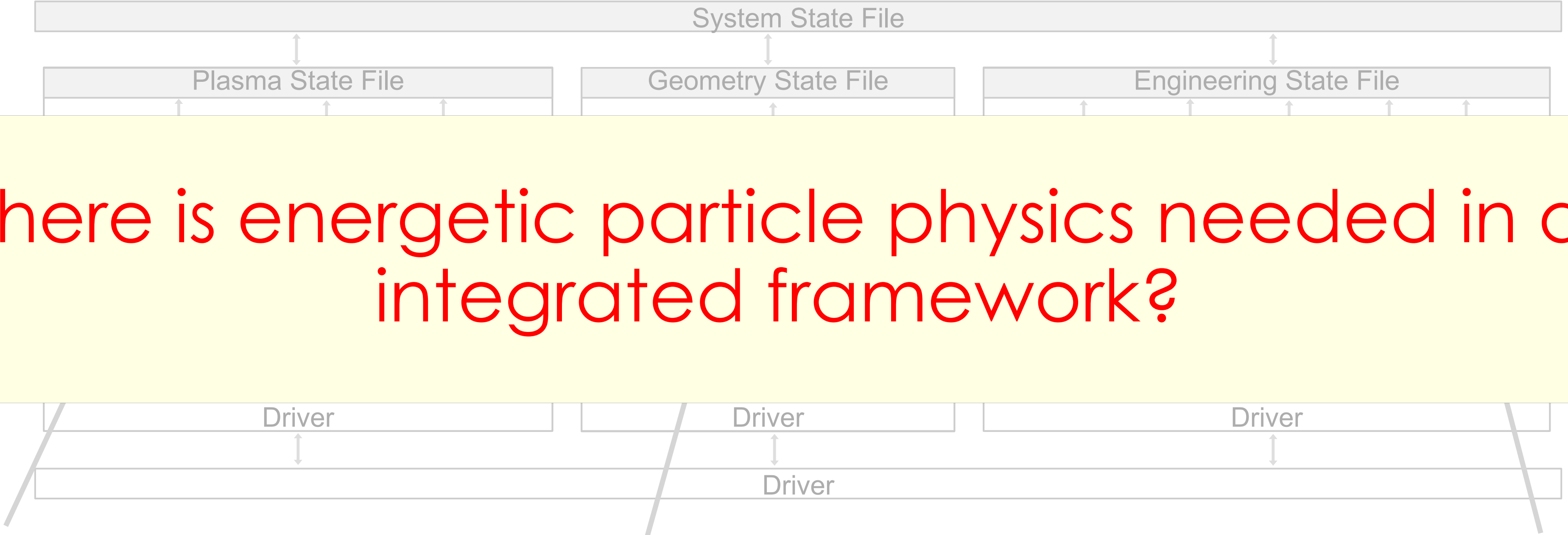
Fusion-Engineering

- Includes Multiphysics simulation tools

Approach: flexible component-based framework & data structure

Framework & Workflow

Capable of integrating swappable modules with diverse CPU/GPU requirements



Where is energetic particle physics needed in an integrated framework?

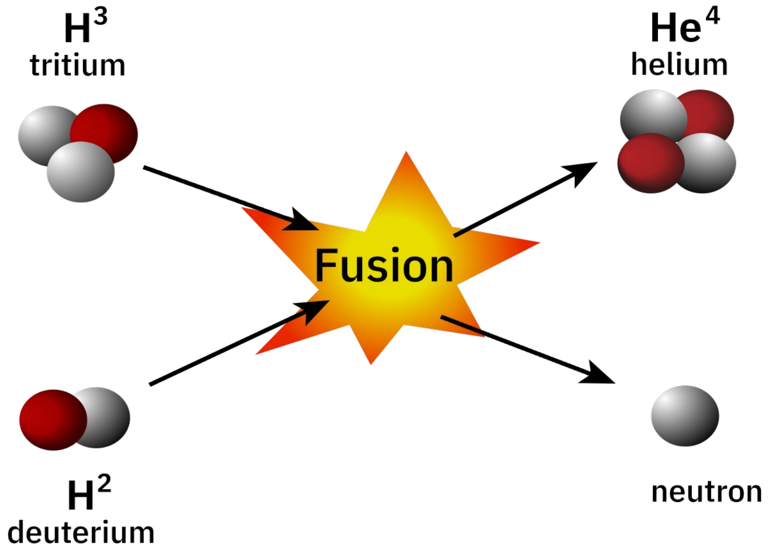
Fusion-Plasma
- Based on the open-source IPS (Integrated Plasma Simulator) developed in AToM SciDAC

Parametric Geometry
- Includes systems codes and parameterized geometry representation

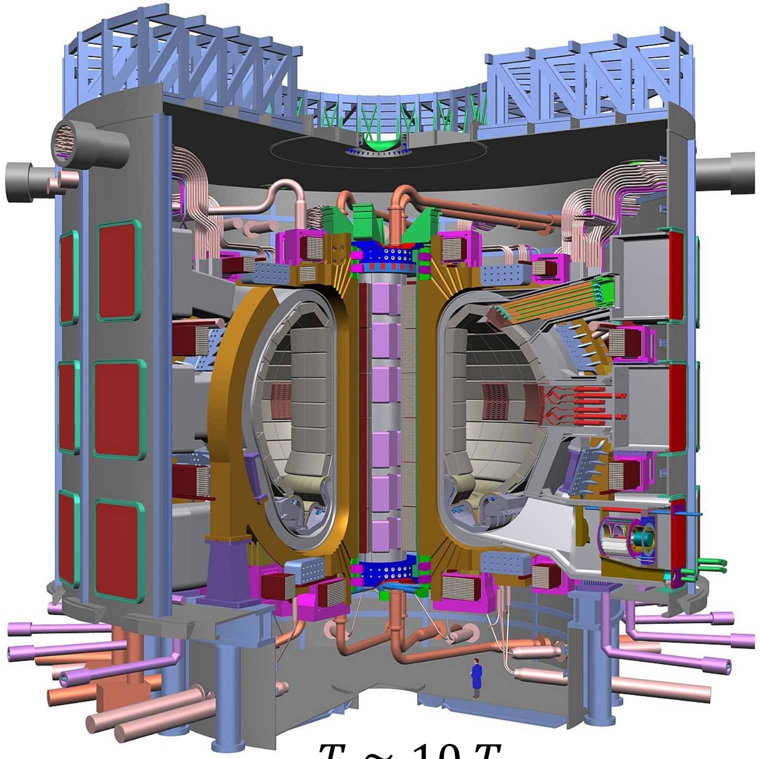
Fusion-Engineering
- Includes multiphysics simulation tools based on Fusion Energy Reactor Models Integrator (FERMI)

Energetic particles have higher temperature in comparison to thermal plasma

3.5MeV



14 MeV



$T \approx 10\, T_{Sun}$

ITER- International Thermonuclear Experimental Reactor

Energetic particle sources:

- Injecting high energy neutral particles (NBI) to heat plasma (NBI).
- energetic alpha particles as by-product of fusion reactions.
- High energy Runaway electrons produced during thermal quench in disruptions or Tritium beta decay

} Alfvén instabilities (NBI, alpha particles)

} Whistler instabilities (runaway electrons)

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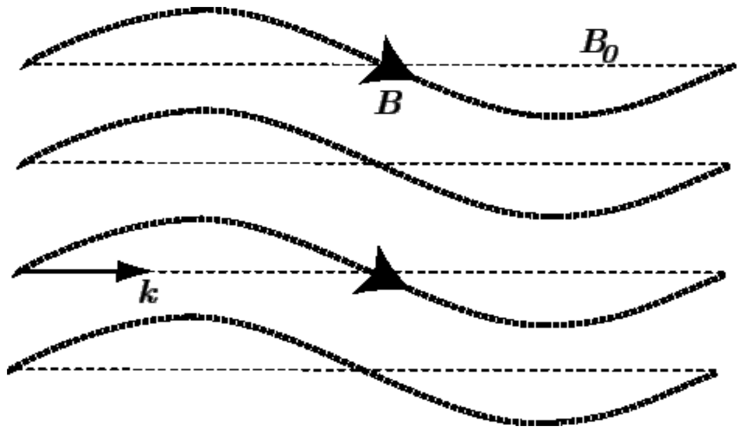
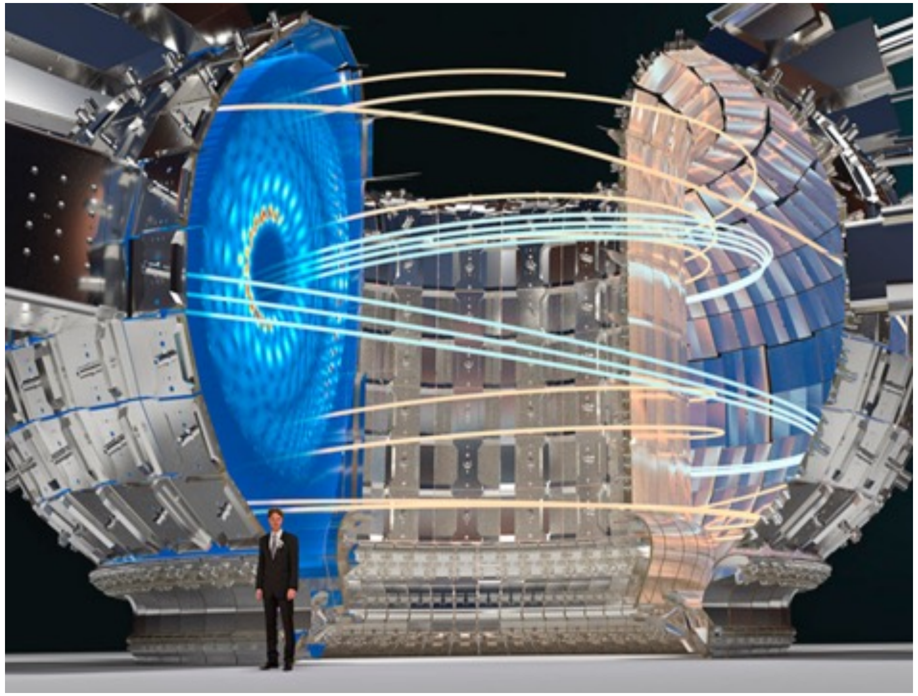
https://www.atomicarchive.com/science/fusion/index.html,

Alfvén waves are transverse electromagnetic waves created by perturbations in the magnetic field lines.

Perturbation



Alfvén eigenmodes in ITER



Alfvén Wave dispersion relation :
$\omega = k_{\parallel} v_A, \quad where \quad v_A = \frac{B}{\sqrt{\mu_0 m_i n_i}}$ is the Alfven speed.

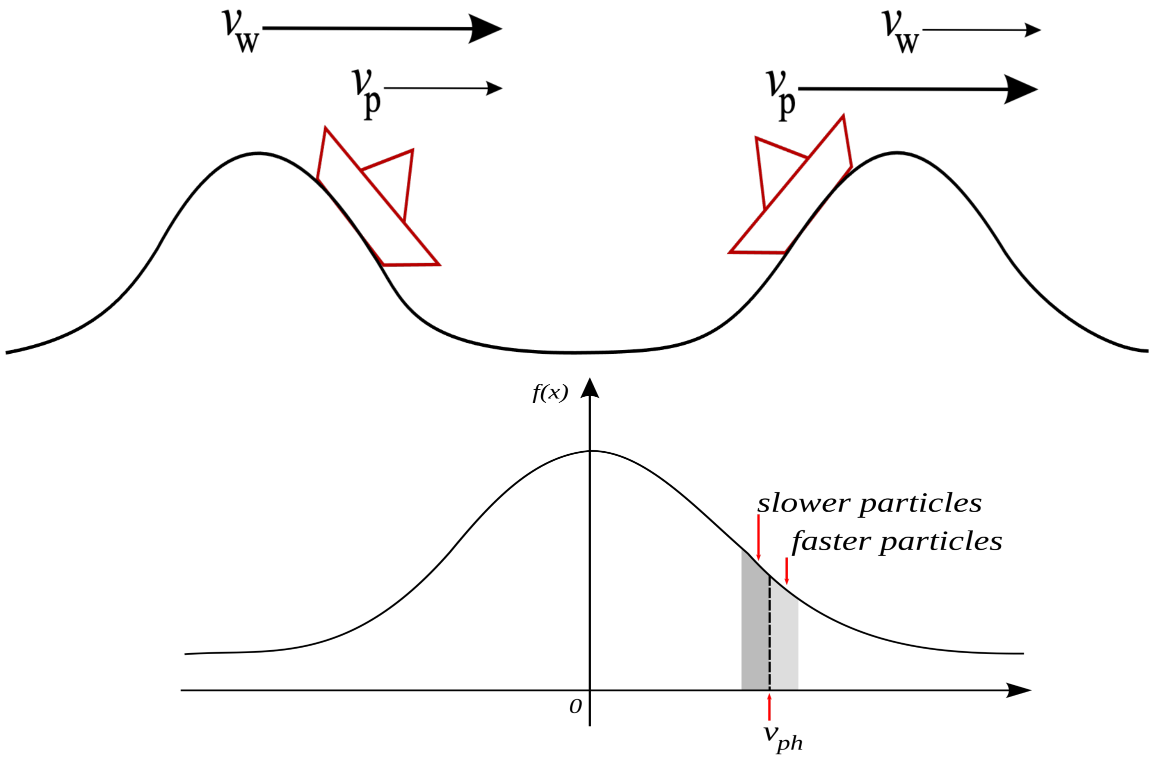
$\omega = |k_{\parallel}| v_{AE}$, where $v_{AE} = \frac{v_A}{4\pi q R}$, $|k_{\parallel}| = \frac{1}{R}\left|n - \frac{m}{q}\right|$

- Alfvén eigenmodes is a special class of Alfvén wave that exist in fusion devices due to periodic boundary conditions imposed by the machine's geometry.

Challenge- Waves may interact resonantly with charged particles and can become unstable

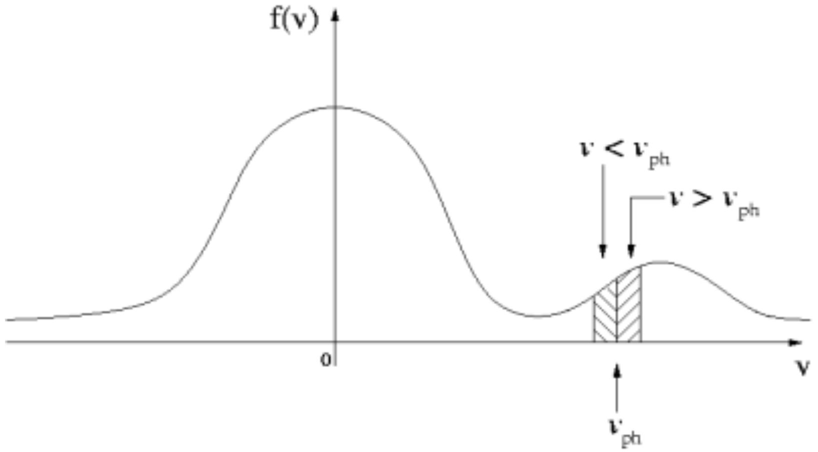
FM radio is tuned to resonate with certain frequencies that correspond to a particular radio station/channel

In plasmas, surfer riding a wave picture demonstrates Landau resonance phenomena between charged particles and plasma waves

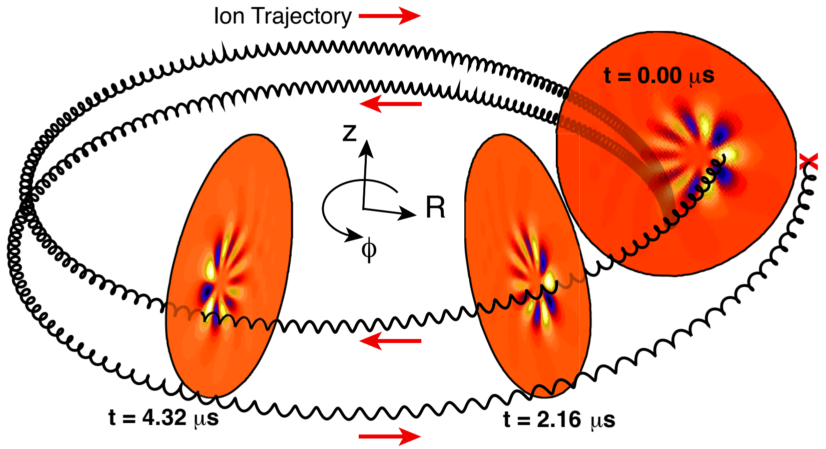


Source: https://en.wikipedia.org/wiki/Landau_damping

How do energetic particles cause Alfvén instabilities?



Bump-on tail distribution cause inverse Landau damping



[Pace, Physics Today (Oct. 2015)]

- Energy exchange can occur via Landau resonance as the ion stays in phase with the wave as it traverses the mode.
- Gradients in real space drive instability,
- Can cause redistribution that affects core performance or loss of fast ions that damage the first wall materials.

Source: https://commons.wikimedia.org/wiki/File:Bump_on_tail_dist.png

[Pace, Physics Today (Oct. 2015)]

To demonstrate an economically viable fusion energy source energetic alpha particle confinement is necessary

	Fusion Gain	α-Heating Fraction	Scientific Frontier
	$Q = \frac{P_{fusion}}{P_{heat}}$	$f_\alpha = \frac{P_\alpha}{P_\alpha + P_{heat}}$	
Scientific Breakeven	Q = 1	17%	Alpha confinement
Burning Plasma Regime	Q = 5	50%	Alpha heating; Alpha effects on energetic particle instabilities
	Q = 10	67%	Strong alpha heating; Non-linear coupling effects
	Q = 20	80%	Burn Control; potentially strong non-linear coupling
	Q = ∞	100%	Ignition

Theoretical Model for FAR3d code

Thermal Plasma

- Reduced MHD equations-
  Ohm's law &
  Vorticity
- Compressibility effects-
  Continuity &
  momentum equation

Energetic Particles

Computationally efficient by truncating moments of gyrokinetic equation with appropriate closures for kinetic effects

- Gyrofluid Model with precise emulations of kinetic effects

FAR3d pseudo-spectral representation

Dynamical (time-evolving) variables:

$$X(\rho,\theta,\zeta)=\sum_{m,n}\left[X_{mnc}(\rho)\cos(m\theta-n\zeta)+X_{mns}(\rho)\sin(m\theta-n\zeta)\right]$$

Equilibrium (steady-state) quantities:

$$E(\rho,\theta,\zeta)=\sum_{m,n}\left[E_{mnc}(\rho)\cos(m\theta)+E_{mns}(\rho)\sin(m\theta)\right]$$

Axisymmetric tokamak

$$E(\rho,\theta,\zeta)=\sum_{m,\hat{n}=\pm iN_{fp}}\left[E_{mnc}(\rho)\cos(m\theta-\hat{n}\zeta)+E_{mns}(\rho)\sin(m\theta-\hat{n}\zeta)\right]$$

Stellarator with field period symmetry (N_{fp} field periods)

Uses finite-differences in the radial direction and Fourier expansions in two angular variables to evolve the dynamic physical variables until convergence is met.

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Structure of FAR3d equations:

$$\mathbf{L}\frac{\partial \vec{y}}{\partial t} = \mathbf{R}\vec{y} + N(\vec{y})$$

Solution vector evolution equations,
N is the nonlinear term

$$\mathbf{L}\frac{\vec{y}^{t+\Delta t} - \vec{y}^{t}}{\Delta t} = \mathbf{R}\frac{\vec{y}^{t+\Delta t} + \vec{y}^{t}}{2}$$

Semi-implicit approximation for N = 0

$$\vec{y}^{t+\Delta t} = \left(\mathbf{L} - \frac{\Delta t}{2}\mathbf{R}\right)^{-1}\left(\mathbf{L} + \frac{\Delta t}{2}\mathbf{R}\right)\vec{y}^{t}$$

Semi-implicit solution for N = 0

- **Degrees of freedom** (size of L, R, y): (number of equations) x radial grid points x number of Fourier modes x 2 Can be 10^5 to 10^6 for linear runs, 5 to 10 times larger for nonlinear runs.

Linear Solver

- The linear system $\vec{y}^{t+\Delta t} = \left(\mathbf{L} - \frac{\Delta t}{2}\mathbf{R}\right)^{-1} \left(\mathbf{L} + \frac{\Delta t}{2}\mathbf{R}\right)\vec{y}^{t}$ is solved at each time step.
- This is done as a two-step process using the direct block tridiagonal solvers CDECBT and CSOLBT developed by Alan Hindmarsh.

L and **R** have bloc-tridiagonal structure:

$$\begin{bmatrix} \mathbf{A} & \mathbf{B} & & & & & & \\ \mathbf{C} & \mathbf{A} & \mathbf{B} & & & & & \\ & \mathbf{C} & \mathbf{A} & \mathbf{B} & & & & \\ & & \mathbf{C} & \mathbf{A} & & & & \\ & & & & \ddots & & & \\ & & & & \mathbf{A} & \mathbf{B} & & \\ & & & & \mathbf{C} & \mathbf{A} & \mathbf{B} & \\ & & & & & \mathbf{C} & \mathbf{A} & \mathbf{B} \\ & & & & & & \mathbf{C} & \mathbf{A} \end{bmatrix}$$

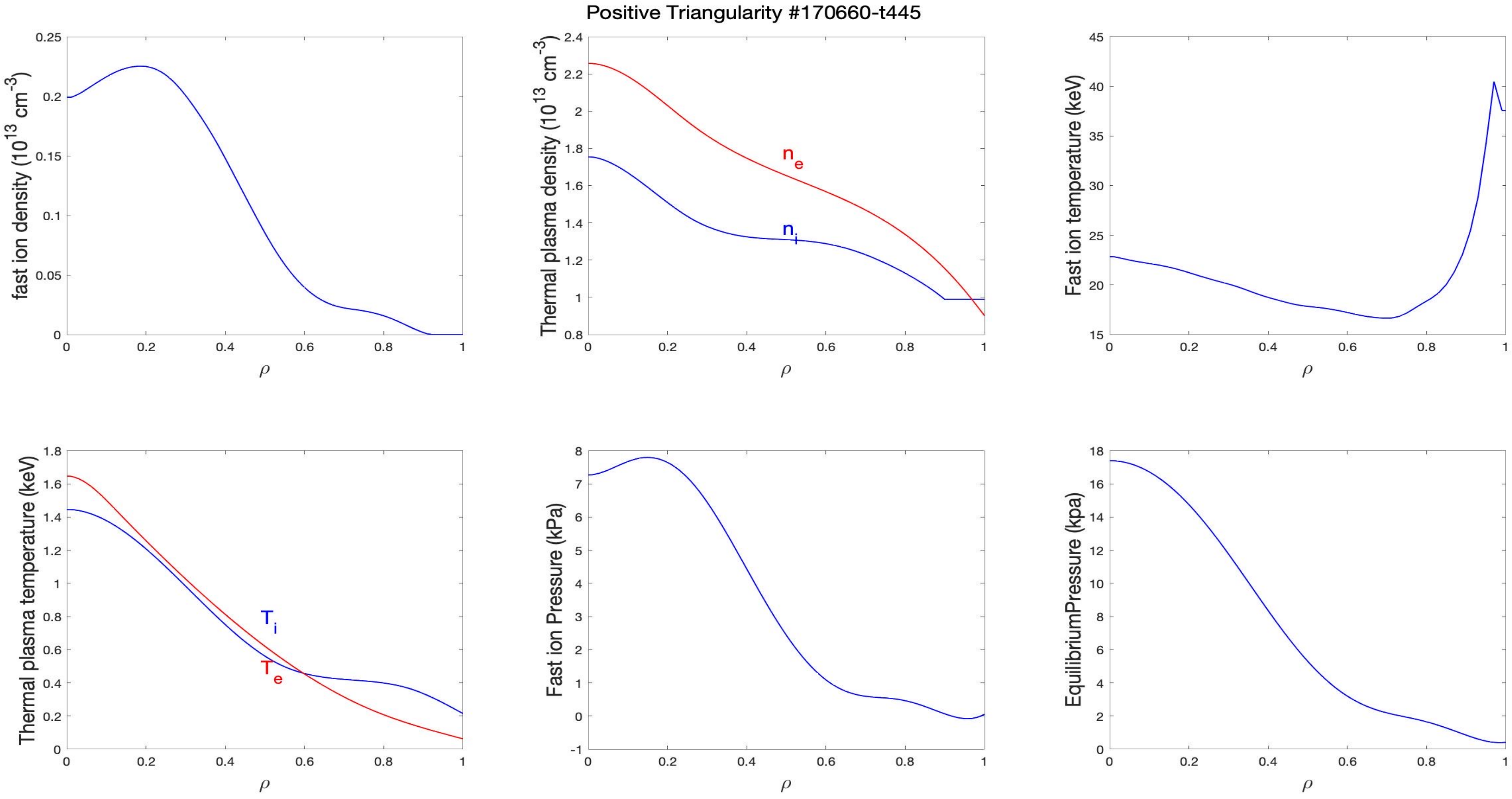
mj block rows = # of radial grid points

A, B, C are square sub-matrices with dimensions of NxN where N = 2 x # Fourier modes x number of equations

- Numerical schemes used: i) a semi-implicit initial value solver which calculates the dominant mode (having the largest growth rate) ii) an eigenvalue solver calculates the stable and unstable (sub-dominant modes).

Alfven eigenmodes observed in DIII-D

- Input profiles:



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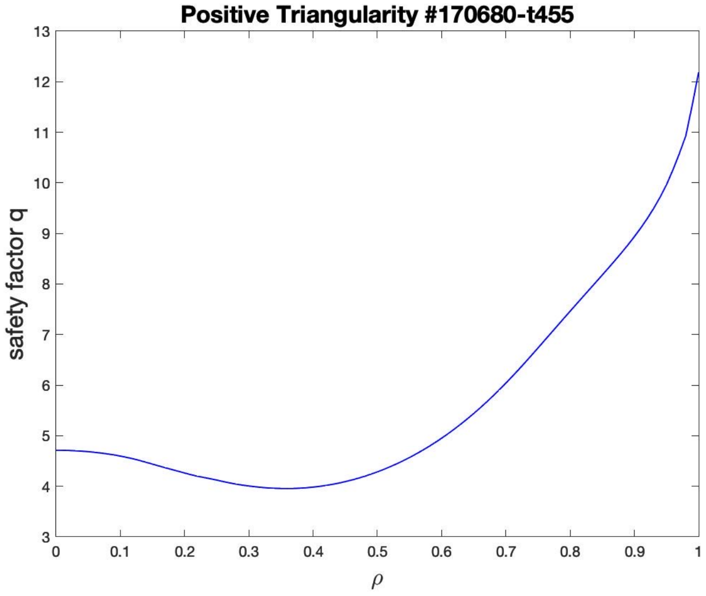
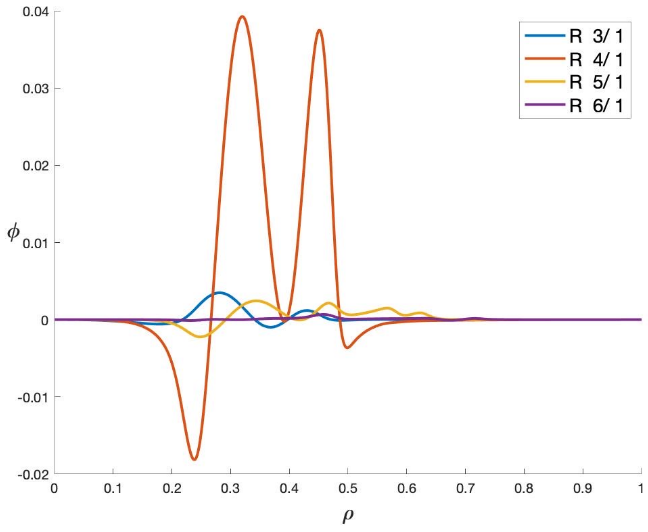
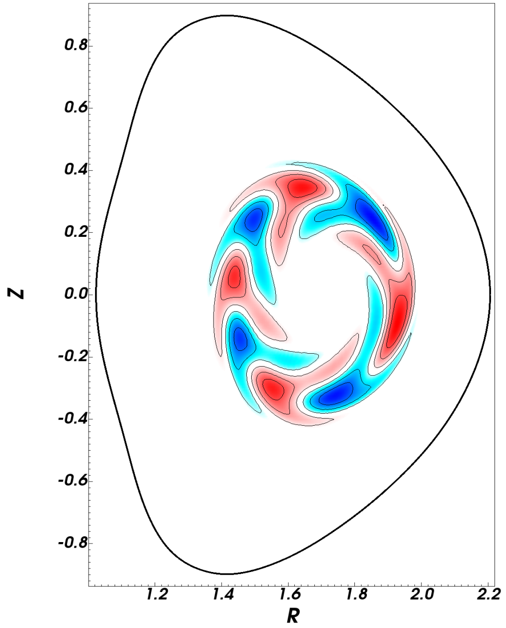
Reversed Shear Alfven Eigenmode (RSAE)





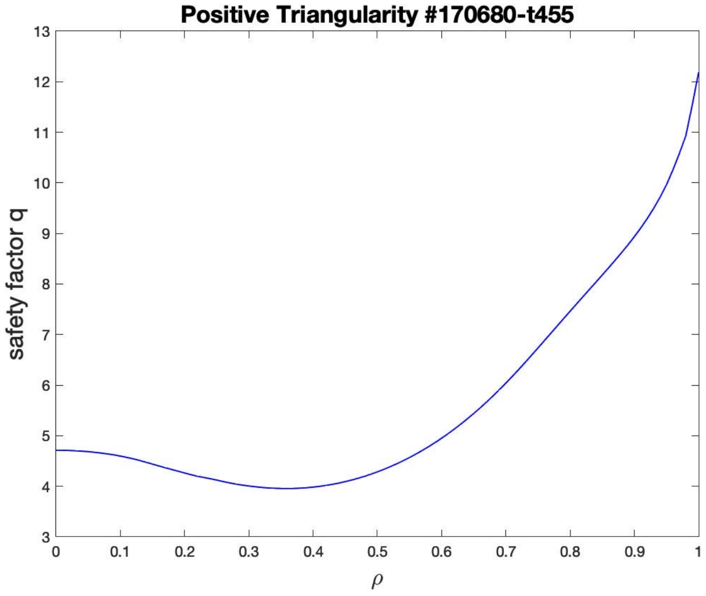
1-D eigenmode plot

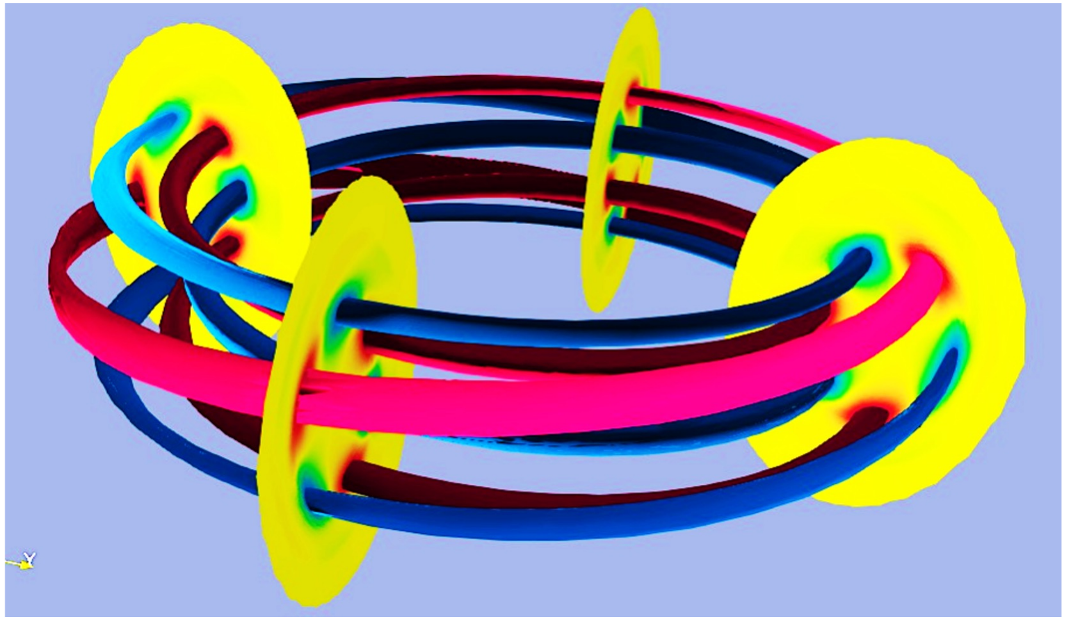


poloidal cros-section plot
2-D eigenmode structure in
DIIID tokamak.

Electrostatic potential eigenfunction plot for n=1 at fast particle beta=0.0042, $v_{th,f}/v_A$=0.14, showing an m=4 RSAE mode with frequency 35 KHz and growth rate=0.011 τ_A^{-1}.

Reversed Shear Alfven Eigenmode (RSAE)





poloidal cros-section plot 3-D eigenmode structure in DIIID tokamak.

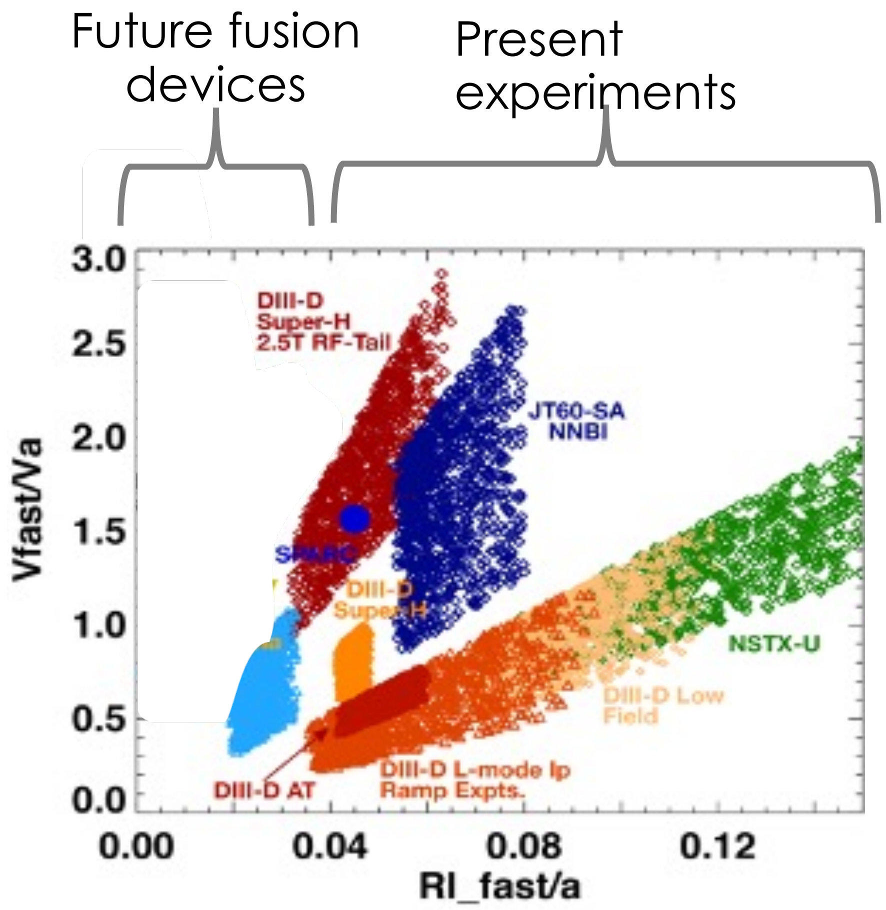
Electrostatic potential eigenfunction plot for n=1 at fast particle beta=0.0042, $v_{th,f}/v_A$=0.14, showing an m=4 RSAE mode with frequency 35 KHz and growth rate=0.011 τ_A^{-1}.

Challenge: Energetic alpha particle transport and losses may limit performance of a reactor-level fusion device

How to study role of alpha particle transport on performance of a reactor-level fusion device?

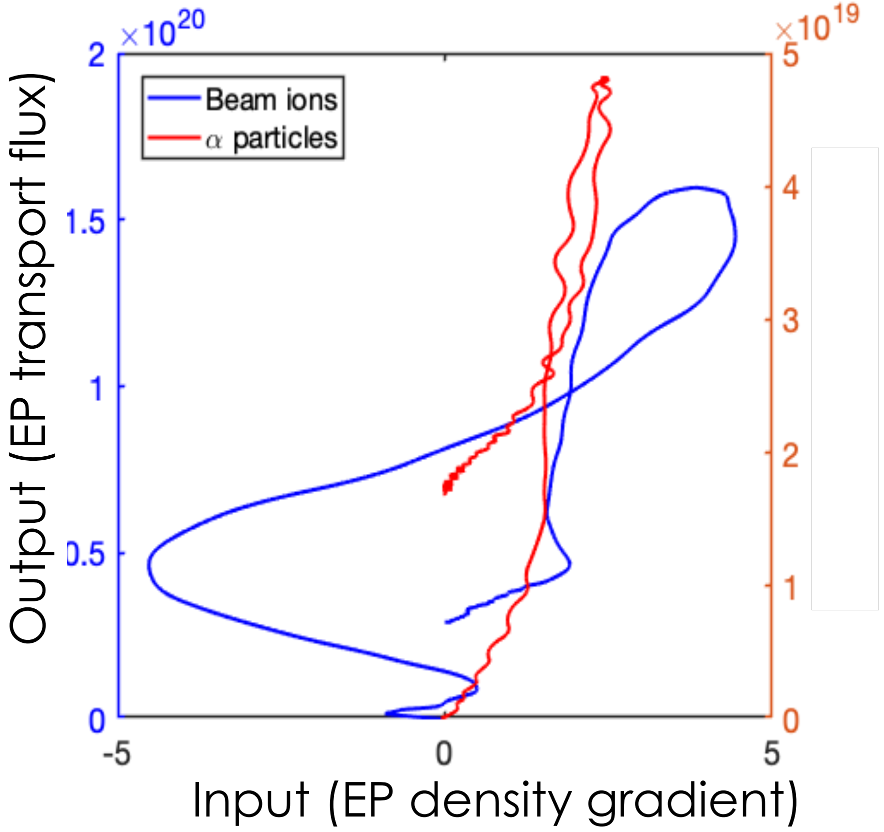
Existing simulation codes **take weeks on supercomputers** to perform calculations of EP transport

Impractical to run in integrated scenarios for FPP design calculations



Goal: Develop a surrogate model of alpha transport using nonlinear FAR3d simulations

- Highly nonlinear transport depends on multiple profiles and parameters
- Need to use techniques such as deep neural networks, transfer learning, etc.



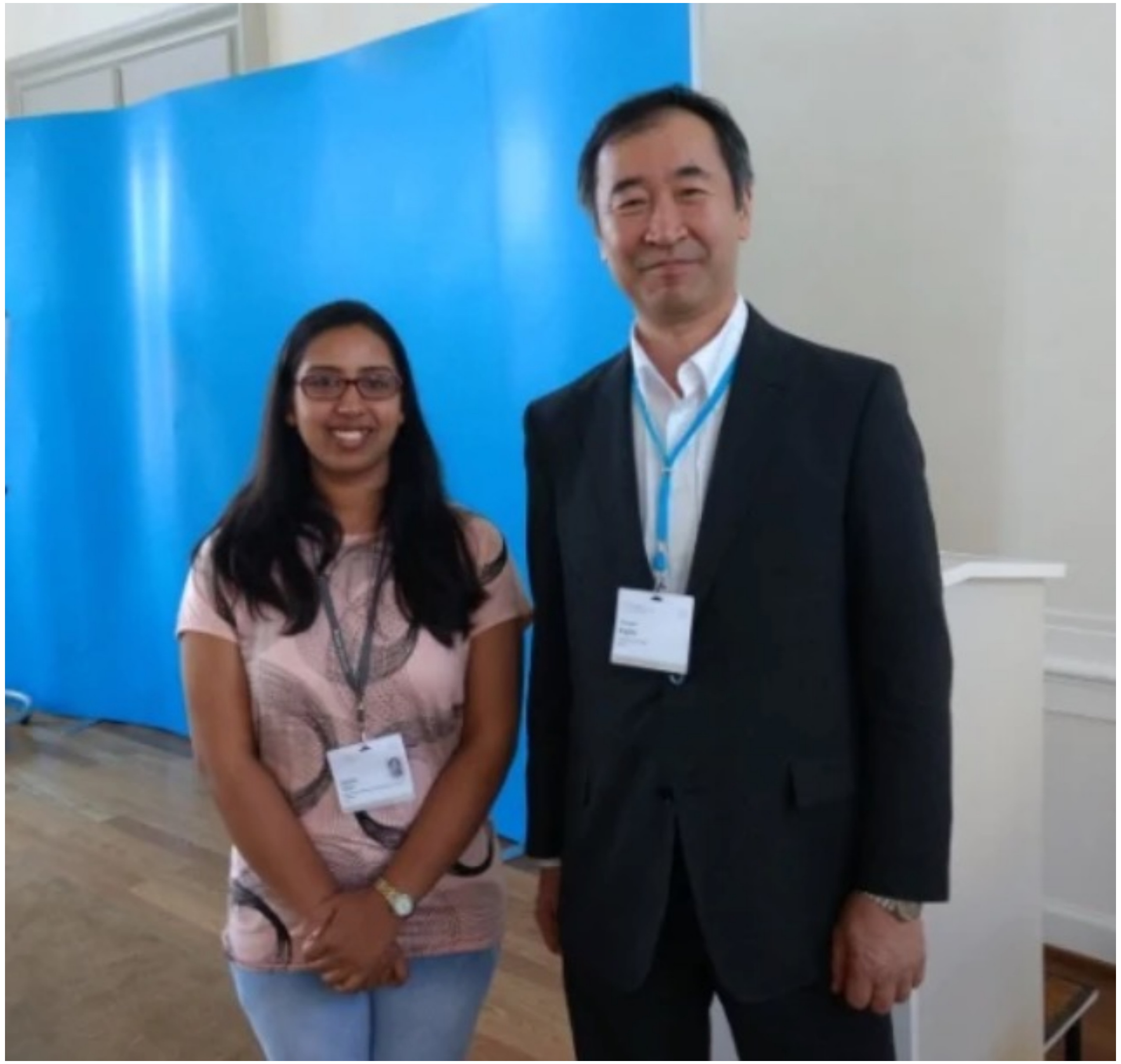
FAR3d simulations of ITER steady state case

- Faster and accurate predictions of EP transport will be included in integrated framework for several applications, viz.
  - Fusion pilot plant design and optimization
  - Real-time prediction of burn control

Key Takeaways

- Different theoretical approaches to describe plasma
  - Fluid, kinetic, MHD, hybrid
- Resonant interactions between energetic particles and plasma waves driven plasma instabilities
- Plasma instabilities can in-turn transport and de-confine energetic particles-can be harmful or useful
- To design a future fusion reactor, we need to couple the physics of different regions of plasma in a single integrated framework- including the alpha particle physics via developing machine learning based surrogates.

Picture with Prof. Takaki Kajita during Lindau meeting



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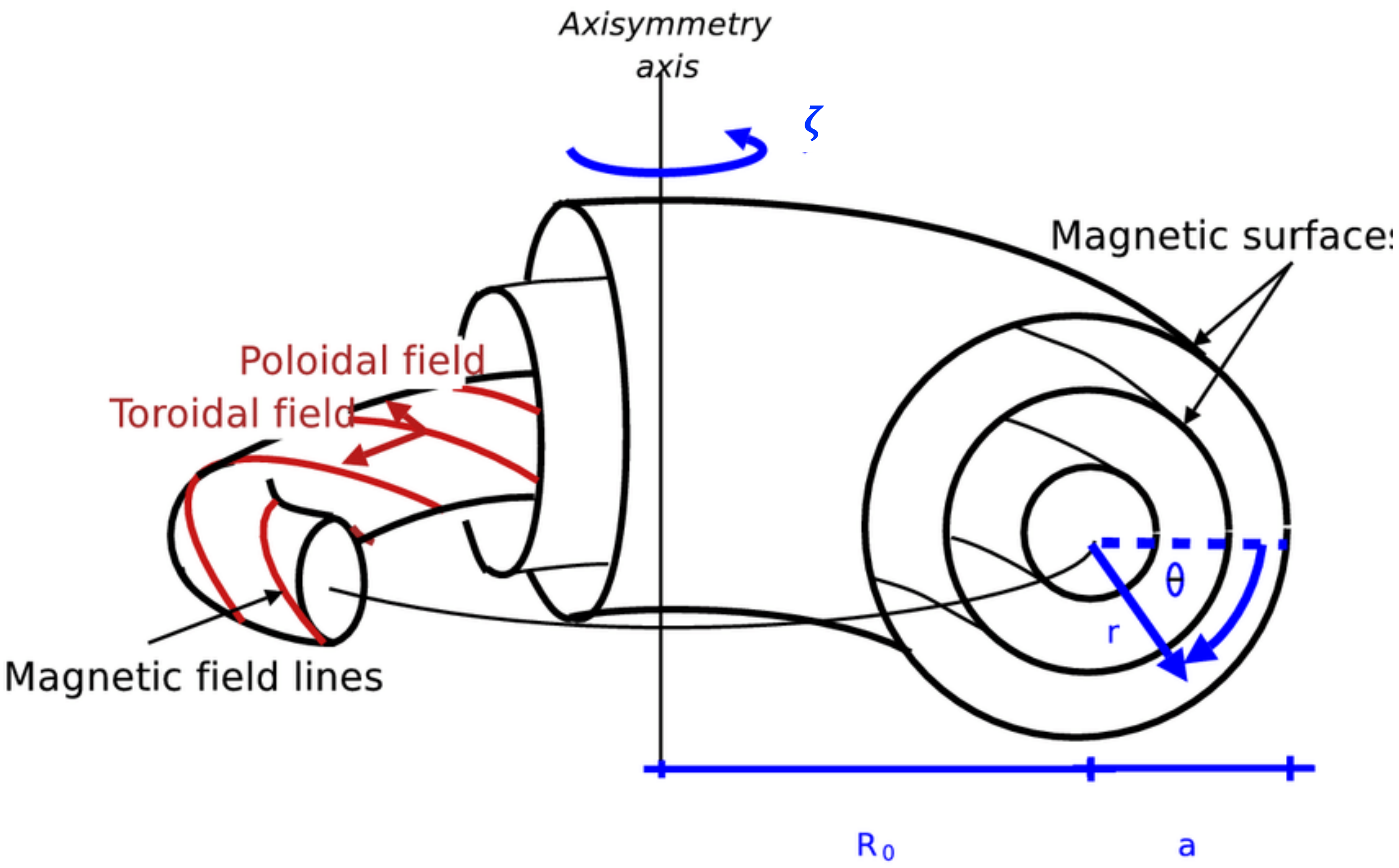
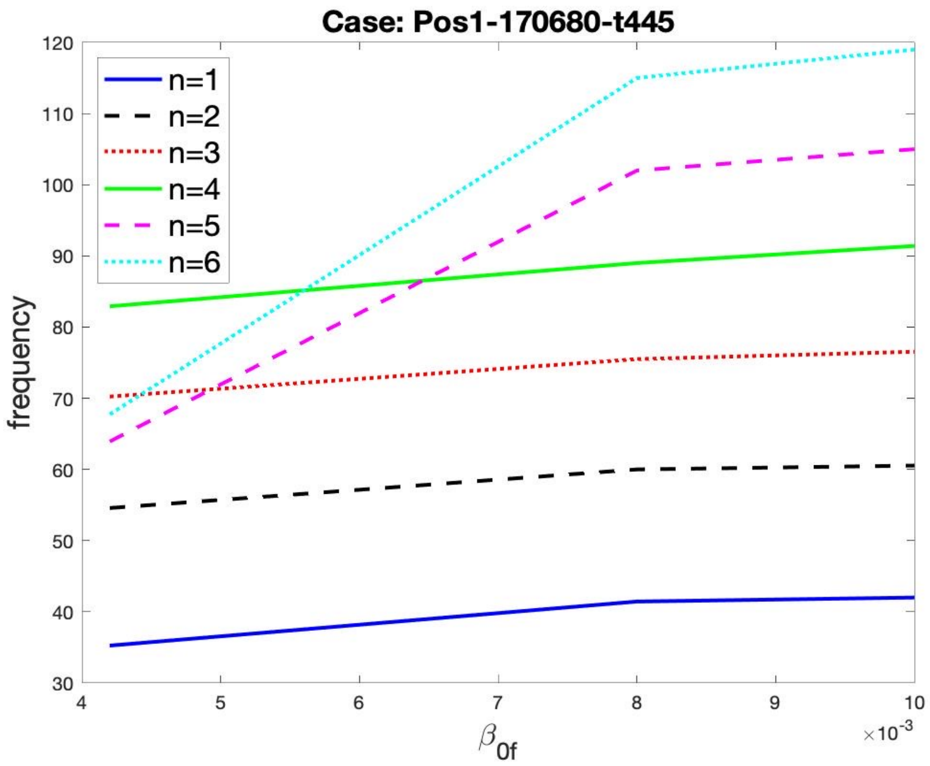
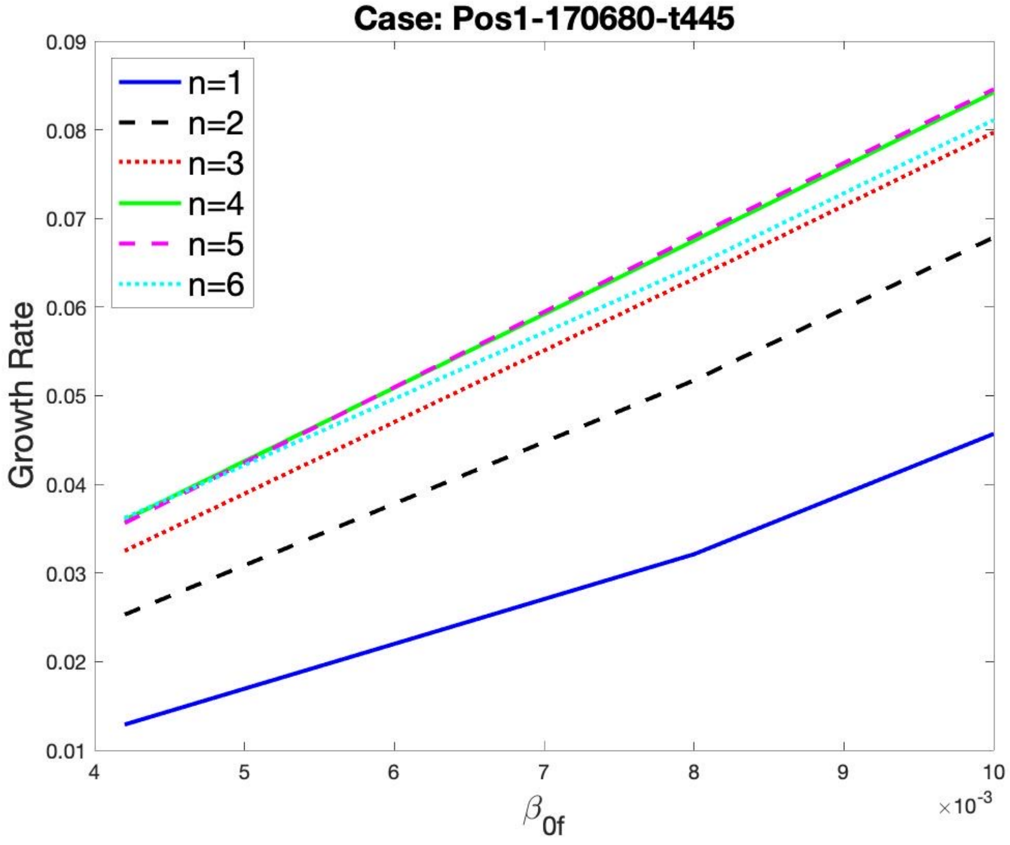
Toroidal coordinates



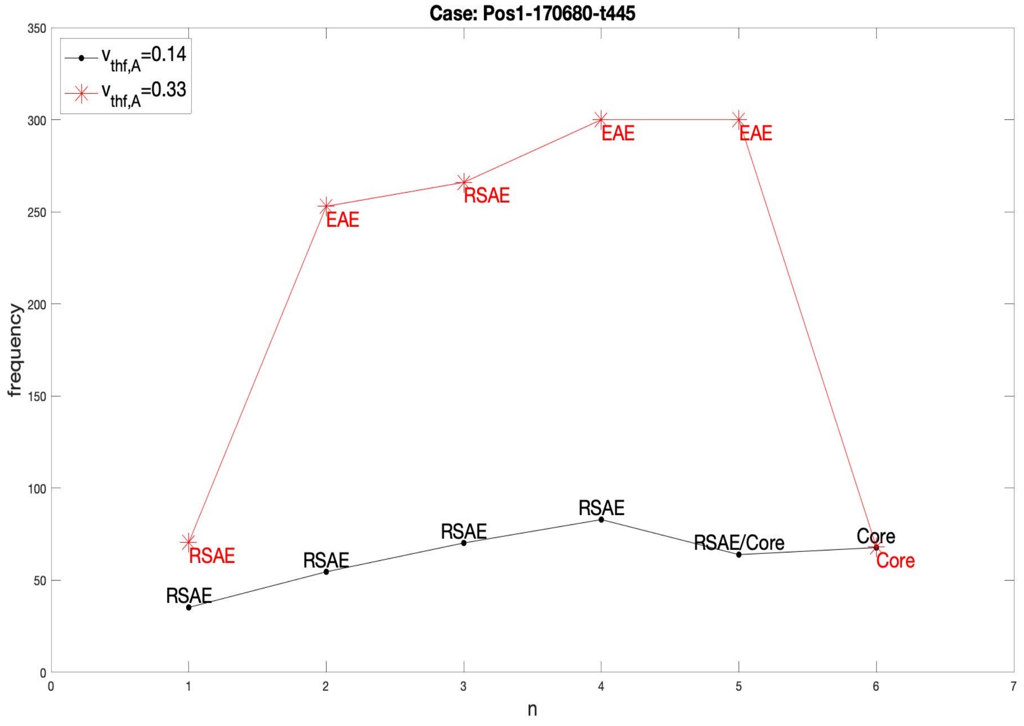
Effect of fast particle β

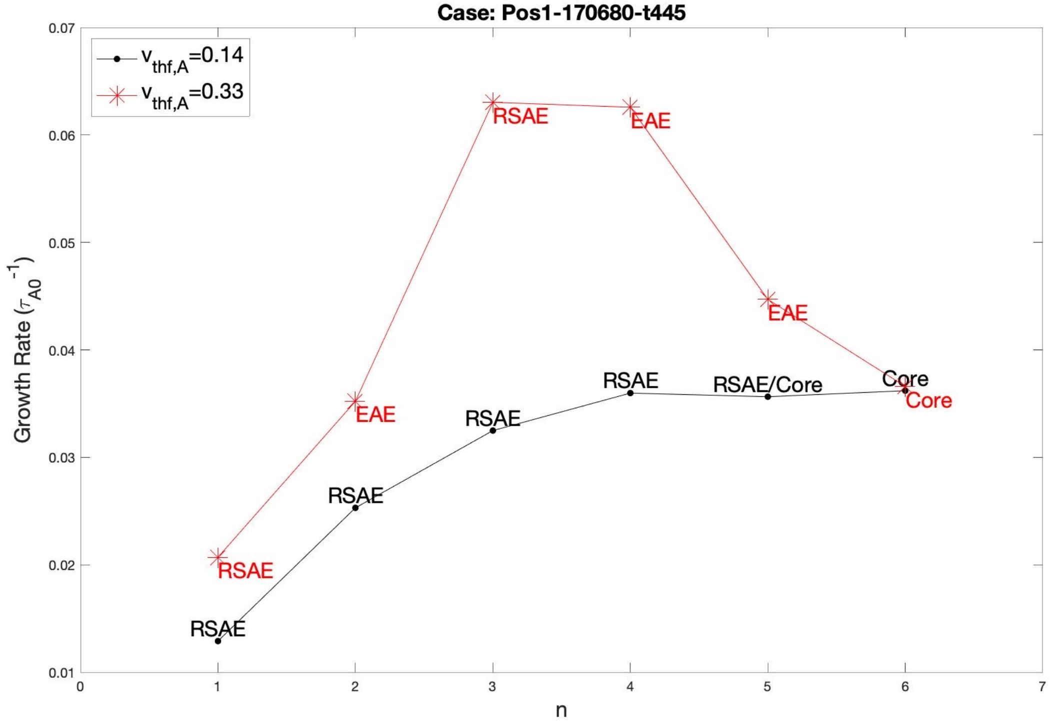




- With increase in fast particle beta, no change in the type of eigenmode is observed.
- However, an increase in growth rate is clearly indicated which due to increase in fast particle pressure and hence increased transfer of energy to Alfven eigenmode.

Effect of fast particle energy via $v_{th,f}/v_A$





- With increase in energy of neutral beam, transition takes place from RSAE to EAE mode.
- An increase in growth rate is observed with increase in beam power and a peak in growth rate is observed for n=4 for which $k_{\perp}\rho \approx 1$.
- A factor governing energy exchange is the alignment of energetic particle orbit with the eigenmode. Extracted energy scales linearly as long as the particle orbit is small compared to radial extent of the mode and Radial extent shrinks with n^{-1} .

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