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M3D-K Simulations of Wave-Particle Interaction with Realistic Fast Ion Distribution

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Initialization with Realistic Fast Ion Distributions could Improve Accuracy of Hybrid simulations

- Fluid/kinetic hybrid simulation codes such as M3D-K typically use a simple analytic form to specify the initial fast ion distribution.
 This could limit the simulation accuracy when the analytic distribution is a poor fit to the actual distribution.
- An interface between the output of tokamak fast ion Monte Carlo code TRANSP/NUBEAM and M3D-K has been developed.
 → More realistic fast ion distributions from NUBEAM can be directly used as M3D-K inputs to improve simulation accuracy.
- M3D-K linear simulations of non-resonant kink mode and TAE mode on NSTX have been performed with analytic and realistic fast ion distributions to validate the new method and check the possible benefits.

M3D-K: Global Kinetic/MHD Hybrid Code

$$\rho \frac{d\mathbf{v}}{dt} + \rho \left(\mathbf{v}_{i}^{*} \cdot \nabla \right) \mathbf{v}_{\perp} = -\nabla \cdot P - \nabla \cdot \mathbf{P}_{h} + \mathbf{J} \times \mathbf{B} - \mathbf{b} \mathbf{b} \cdot \nabla \cdot \prod_{i}$$
$$\mathbf{P}_{h} = P_{\perp} \mathbf{I} + \left(P_{\parallel} - P_{\perp} \right) \mathbf{b} \mathbf{b}$$

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}_i) = 0$$

$$\rho \left[\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} + (\mathbf{v}_i^* \cdot \nabla) \mathbf{v}_{\perp} \right] = -\nabla \mathbf{p} + \mathbf{J} \times \mathbf{B} + \mu \nabla^2 \mathbf{v}$$

$$\mathbf{E} + \mathbf{v} \times \mathbf{B} = \eta \mathbf{J} - \frac{\nabla_{\parallel} p_e}{ne}$$

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

Extended MHD equations (Single fluid, Two-fluid (but not used in this work))

>Hybrid (Kinetic fast ions)

Kinetic fast ions couple back to fluid model through pressure tensor, which is calculated by gyrokinetic or driftkinetic equation

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

$$\begin{split} \frac{\partial p}{\partial t} + \mathbf{v} \cdot \nabla p &= -\gamma p \nabla \cdot \mathbf{v} + \nabla \cdot n \chi_{\perp} \nabla \left(\frac{p}{\rho}\right) - \mathbf{v}_{i}^{*} \cdot \nabla p - \gamma p \nabla \cdot \mathbf{v}_{i}^{*} + \frac{\mathbf{J} \cdot \nabla p_{e}}{ne} + \gamma p_{e} \mathbf{J} \cdot \nabla \left(\frac{1}{ne}\right) \\ \frac{\partial p_{e}}{\partial t} + \mathbf{v} \cdot \nabla p_{e} &= -\gamma p_{e} \nabla \cdot \mathbf{v} + \nabla \cdot n \chi_{\perp e} \nabla \left(\frac{p_{e}}{\rho}\right) + \frac{\mathbf{J}_{\parallel} \cdot \nabla p_{e}}{ne} - \gamma p_{e} \nabla \cdot \left(\mathbf{v}_{e}^{*} - \frac{\mathbf{J}_{\parallel}}{ne}\right) \\ \mathbf{where} \qquad \mathbf{v}_{e}^{*} &= -\frac{\mathbf{B} \times \nabla p_{e}}{neB^{2}}, \quad \mathbf{v} \equiv \mathbf{v}_{i} - \mathbf{v}_{i}^{*} = \mathbf{v}_{e} - \mathbf{v}_{e}^{*} + \frac{\mathbf{J}_{\parallel}}{ne} \qquad \mathbf{v}_{i}^{*} \equiv \mathbf{v}_{e}^{*} + \frac{\mathbf{J}_{\perp}}{ne}, \qquad *Fu \end{split}$$

*Fu et al. Phys. Plasmas 2006

Main Features of M3D-K

- ➤Use realistic geometry
- ➤Use experimental parameters and profiles
- ≻Global
- Linear and nonlinear
- ➢Non-perturbative fast ion effects (i.e., can model EPM)
- Numerical equilibrium calculation with plasma rotation and anisotropic fast ion pressure
- Interface with TRANSP/NUBEAM fast ion distribution is developed and tested.



Numerical Fast Ion Distribution is Calculated by Monte Carlo Modeling NUBEAM

>NUBEAM module in TRANSP: a Monte Carlo code for 4D (R,Z, $\lambda = v_{\parallel}/v$, E)

time dependent simulation of fast ion transport in tokamak devices.

Assume fast ions behave classically; could add anomalous radial diffusion operator based on user provided diffusivities

>Includes guiding center drift orbiting, collisional, and atomic physics effects



Fast Ion Distribution Needed to be Transformed from (R,Z,λ,E) to Constants-of-Motion Space

>M3D-K code needs fast ion distribution $f(R,Z,\lambda,E)$ expressed in terms of constants of the motion (P_{ϕ} , μ , E) and the function must be smooth enough to allow derivatives to be taken with E and toroidal angular momentum P_{ϕ} >In addition to P_{ϕ} , μ , E, the sign of v_{\parallel} is also needed to resolve orbit type. >NUBEAM calculated fast ion distribution $f(R,Z,\lambda,E)$ needs to be transformed to $f(P_{\phi}, \mu, E)$ coordinates.

$$\int f(x, y, z, vx, vy, vz) d^{3}\mathbf{x} d^{3}\mathbf{v} \qquad \text{where}$$

$$= \int f(R, Z, \lambda, E) R \sqrt{E} dR dZ d\lambda dE \qquad P_{\varphi} = (eA_{\varphi} + mv_{\varphi})R \approx e \psi(R, Z) + mv_{\parallel}R \frac{B_{\varphi}(R, Z)}{B(R, Z)}$$

$$= \sum_{v_{sign}} \int f_{v_{sign}}(P_{\varphi}, \mu, E) \mathfrak{I}_{v_{sign}}(P_{\varphi}, \mu, E) dP_{\varphi} d\mu dE \qquad \mu = \frac{\frac{1}{2}mv_{\perp}^{2}}{B} = \frac{[1 - (v_{\parallel}/v)^{2}]E}{B(R, Z)} \qquad \lambda = v_{\parallel}/v$$

>Use TRANSP "Plasma State" utility to get ψ and B at each particle location (R,Z), and then calculate P_{ϕ} , μ

Jacobian of the Transform Strongly Depends on Particle Orbit Topology

counter-current Jacobian of the transform from $(R, Z, v_{\perp}^2, v_{\parallel})$ to (P_{φ}, μ, E)



Trapped/passing boundary

Jacobian of the Transform is Calculated by Monte Carlo Method

 $\int f(x, y, z, vx, vy, vz) d^3 \mathbf{x} d^3 \mathbf{v} = \int f(R, Z, \lambda, E) R \sqrt{E} dR dZ d\lambda dE = \sum_{v_{sign}} \int f_{v_{sign}}(P_{\varphi}, \mu, E) \mathfrak{I}_{v_{sign}}(P_{\varphi}, \mu, E) dP_{\varphi} d\mu dE$

>An exact analytic $\mathfrak{T}_{v_{sign}}(P_{\varphi}, \mu, E)$ cannot be calculated because it requires integration over phase space orbits.

≻A Monte Carlo approach is used to calculate Jacobian

≻Procedure:

(1)Generate a large population of ~50 million particles uniformly in phase space (R,Z, λ ,E), within the same range as in the NUBEAM distribution (2)Transform coordinates to constants-of-motion space (3)Bin the particles in (P_{\alphi}, \mu, E) space for each v_{||} sign. (4)The particle number in each (P_{\alphi}, \mu, E) bin proportional to $\Im_{v_{sign}}(P_{\alphi}, \mu, E)$

Constructing Fast Ion Density Function in Constantsof-Motion Space

- >Divide NUBEAM output particle data into two subsets based on v_{\parallel} sign
- >For each subset, sort particles by μ and divide them into several subpopulations of equal width in μ .
- >Divide each subpopulation into a number of bins in the P_{ϕ} and E directions. The bin width in P_{ϕ} and E direction are the same for each subpopulation.
- >Multiply by the numerically calculated Jacobian.
- > Apply Gaussian smoothing in both P_{ϕ} and E directions.
- ➢Fit 2D cubit B-spline to the smoothed data using GSL routines, with uniform knots and a number of coefficient s in each direction approximately 5/8 the number of bins.
- Store the spline coefficients in a file, which can be used to construct fast ion density function in constants-of-motion space and perform quick spline and derivative interpolations at arbitrary location.
- ➤ *Improved from the work of Breslau et al. Sherwood Meeting 2011

Good Agreement between Raw Fast Ion Density Function and Spline Fit in Constants-of-motion Space



🔘 NSTX-U

Gradients are Smooth, Match well with NUBEAM Raw Data



Reconstructed from cubic B-spline fit

 $\frac{\partial f_{co-current}(P_{\varphi}, E, \mu)}{\partial P_{\varphi}}$

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Gradients are Smooth, Match well with NUBEAM Raw Data



Reconstructed from cubic B-spline fit



 $\frac{\partial f_{co-current}(P_{\varphi}, E, \mu)}{\partial E}$

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Gradients are Smooth, Match well with Raw Data (cont'd)



M3D-K Linear Simulations of Non-Resonant Kink Mode on NSTX



Both experiments and simulations show that (1,1) non-resonant kink mode is unstable in NSTX when the shear is low and central safety factor is close but greater than one.

➤The mode is a pressure-driven mode. It can saturate nonlinearly and persist, and can develop m=2 magnetic islands.

>The mode could severely impact performance: flatten rotation, redistribute fast ions, trigger neoclassical tearing modes.

*S. Gerhardt Nucl. Fusion 2011; J. Breslau Nucl. Fusion 2011; F. Wang Sherwood Meeting 2012

>NSTX #124379 at t=0.635s equilibrium profiles >R=0.86m, a=0.6m, B_t(0)=0.44T, n_e(0)=9.3x10¹³cm⁻³ > q_{min} =1.055, $\beta_{thermal}$ (0)=24%, β_{fi} (0)=5%



Reasonable M3D-K Simulations Results Obtained with both Analytic and NUBEAM Fast Ion Distributions



> $\beta_{\text{thermal}}(0)=24\%$ fixed in all cases, $\beta_{fi}(0)/\beta_{tot}(0)==5\%$ for the cases with fast ions; >Fast ions weakly stabilize non-resonant kink mode, and induce mode rotation; >Different fast ion distributions can change mode growth rate and mode frequency.

Initial Analytic & NUBEAM Fast Ion Distributions are Different, and they remain Unchanged during Linear Simulation



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Previous M3D-K Linear Simulations Qualitativity Agree with Experimental Measurements



 Equilibrium and plasma profiles at t=470ms are used as M3D-K inputs.
 Previous M3D-K linear simulation results (Fu TTF 2011) are similar to the measurements with respect to mode frequency, core-localized radial structure, and phase shift, but there is a significant radial shift between M3D-K simulations and measurements from multichannel reflectometer.



Parameters and Profiles for M3D-K Simulation of n=3 TAE on NSTX



🔘 NSTX-U

Similar Mode Structure Obtained with Analytic and NUBEAM Fast Ion Distributions



 $\gamma/\omega_{A} = 4.7\%$, f=110kHz

Detailed Mode Structure Affected by Initial Fast Ion Distribution





Comparison of Analytic and NUBEAM Fast Ion Distributions



Conclusions and Future Plan

- An interface between NUBEAM output and M3D-K has been developed and tested. More realistic NUBEAM fast ion distribution now can be used as M3D-K inputs to improve simulation accuracy.
- M3D-K linear simulation of non-resonant kink mode on NSTX show that fast ions can weakly stabilize the mode. Different fast ion distributions (analytic distribution and NUBEAM fast ion distribution) can affect mode growth rate and frequency.
- Preliminary simulation results of n=3 TAE mode with NUBEAM fast ion distribution are similar to previous results with analytic fast ion distribution. But detailed mode structure and frequency are affected by the input NUBEAM fast ion distribution.
- Future work
- Improve the accuracy of Jacobian calculation near the confined/lost boundary, trapped and passing bounday
- Convergence study and plasma parameter scan for n=3 TAE case
- Compare mode structure with reflectometer measurements and NOVA-K results