A solver for energetic particle transport in constants of motion space with collision and phase space zonal structures in tokamak plasmas

MAX-PLANCK-INSTITUT FÜR PLASMAPHYSIK

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Abstract

Recently, a general theoretical framework for the transport of Phase Space Zonal Structures (PSZS) has been developed [1,2]. PSZS are the long-lived toroidal symmetric ($n = 0$) structures that define the nonlinear equilibrium in the presence of fluctuations such as Alfvenic instabilities. In order to include sources and sinks and collisional slowing down processes, a new solver, ATEP-3D was implemented to describe the evolution of the EP distribution in the 3D Constants of Motion (CoM) space. It is fully embedded in ITER IMAS framework and combined with the LIGKA/HAGIS codes [3,4]. The new development is motivated by the need to use the CoM representation in the PSZS transport model. The Fokker-Planck collision operator represented in the 3D CoM space is derived and implemented in the HAGIS code giving orbit-averaged collisional coefficients. For solving the PSZS equation including collisions, a finite volume method and the implicit scheme are adopted in the ATEP-3D code for optimized numerical properties. Open boundary conditions that allow the flux to pass through the boundaries without affecting the interior solution are implemented. ATEP-3D allows the analysis of the particle and power balance with sources and sinks in the presence of EP transport induced by Alfvenic fluctuations to evaluate the EP confinement properties.

Advanced Transport modelling (ATEP): for multi-scale modelling of EP transport

- Multiple spatial-temporal scales in EP transport requires advanced transport modeling
  - Spatial scales: EP orbit width $\sim 0.1a$ related to EP energy (meso-scale between device size & ρ_i)
  - Temporal scales: AE excitation, nonlinear wave-particle, wave-wave interactions, EP transport
  - Present 1D local radial transport models are more suitable for thermal ions/electrons
- Constants of Motion: proper description of EP distribution; EP transport model in CoM space is needed→PSZS theory
  - Collisional transport (Neoclassical)
    - Collision: slowing down and diffusion process; Global, Slow (long time scale transport)
  - Wave-induced transport (Collisionless)
    - EP-AE: characteristic velocities of EPs ~ phase velocities of AE
- PSZS (Phase space zonal structure): long-lived toroidal symmetric (n=0) structures
  - AE induced PSZS: Resonant structures, localized
  - General framework established for GK theory of transport, PSZS dynamics due to fluctuations
- ITER IMAS (Integrated Modelling & Analysis System), IDSs as flexible coupling framework

[Lauber 2023EFTC talk; Zonca NJP2015; Falessi & Zonca, POP2018; Falessi & Zonca, POP2019; IMAS https://imas.iter.org]

Partial Differential Equation Solved in the ATEP-3D

- **PSZS transport theory**
  [M. Falessi arXiv:2306.08642]

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

- **PDE solved by ATEP-3D:**

$$\boxed{\frac{\partial f}{\partial t} = C(f) + S + fluctuation\ induced\ transport}$$

- EP distribution function: $f(\boldsymbol{X}, t)$
- Constants Of Motion phase space: $\boldsymbol{X} = (P_\zeta, E, \Lambda)$, where $\Lambda = \mu B_0/\mathrm{E}$, toroidal canonical momentum P_ζ, energy E, and magnetic moment μ
- Source/Sink: $S(\boldsymbol{X}, t)$
- Collision ($\boldsymbol{C}$): Collisional coefficients are numerically calculated by HAGIS.
  - The guiding center particle code HAGIS is implemented with a Monte Carlo model of pitch-angle scattering which includes conservation of momentum [A. Bergmann, POP2001]. HAGIS with collision is validated and applied to studies of bootstrap current and neoclassical transport.

Constructing the collision operator for use in the PSZS theory

$$C(f) = \frac{\partial}{\partial P_\zeta}(D_P f) + \frac{\partial}{\partial E}(D_E f) + \frac{\partial}{\partial \Lambda}(D_\Lambda f) + \frac{\partial^2}{\partial P_\zeta^2}(D_{PP} f) + \frac{\partial^2}{\partial E^2}(D_{EE} f) + \frac{\partial^2}{\partial \Lambda^2}(D_{\Lambda\Lambda} f).$$

- Advection

$$D_{P_\zeta} = \frac{mg}{B}\nu_{s\parallel},$$
$$D_E = mv_\parallel \nu_{s\parallel} + \frac{m}{2}\nu_{s\perp},$$
$$D_\Lambda = -2\Lambda\frac{v_\parallel}{v^2}\nu_{s\parallel} + \frac{1}{v^2}\left(\frac{B_0}{B} - \Lambda\right)\nu_{s\perp},$$

- Diffusion

$$D_{PP} = \frac{m^2 g^2}{2B^2}\nu_\parallel$$
$$D_{EE} = \frac{m^2 v_\parallel}{2}\nu_{\parallel\perp} + \frac{m^2 v_\parallel^2}{2}\nu_\parallel + \frac{m^2}{8}\nu_\perp$$
$$D_{\Lambda\Lambda} = -2\Lambda\frac{v_\parallel}{v^4}\left(\frac{B_0}{B} - \Lambda\right)\nu_{\parallel\perp} + 2\Lambda^2\frac{v_\parallel^2}{v^4}\nu_\parallel + \frac{1}{2v^4}\left(\frac{B_0}{B} - \Lambda\right)^2\nu_\perp.$$

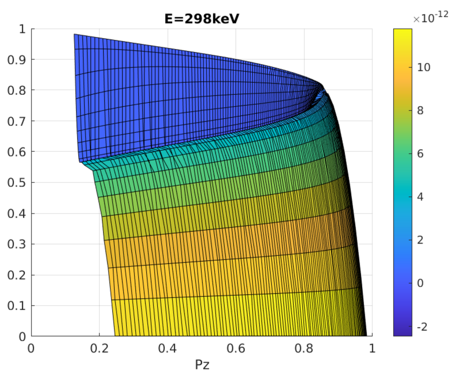
- **Bounce average: finite orbit width effect is included (EP-i/e collisions Banana regime)**
- **Averaged over unperturbed orbit** $\langle D\rangle = \frac{1}{\tau_b}\int D\, dt$**, where** τ_b **is the time of a particle completing its poloidal orbit**

Off-diagonal terms not shown in Eq are omitted currently; Further: full collision operator using Rosenbluth potentials [Lu, Meng, Chankin et al.], non-Maxwellian distribution, collision of EP-EP

Collision coefficients in CoM space

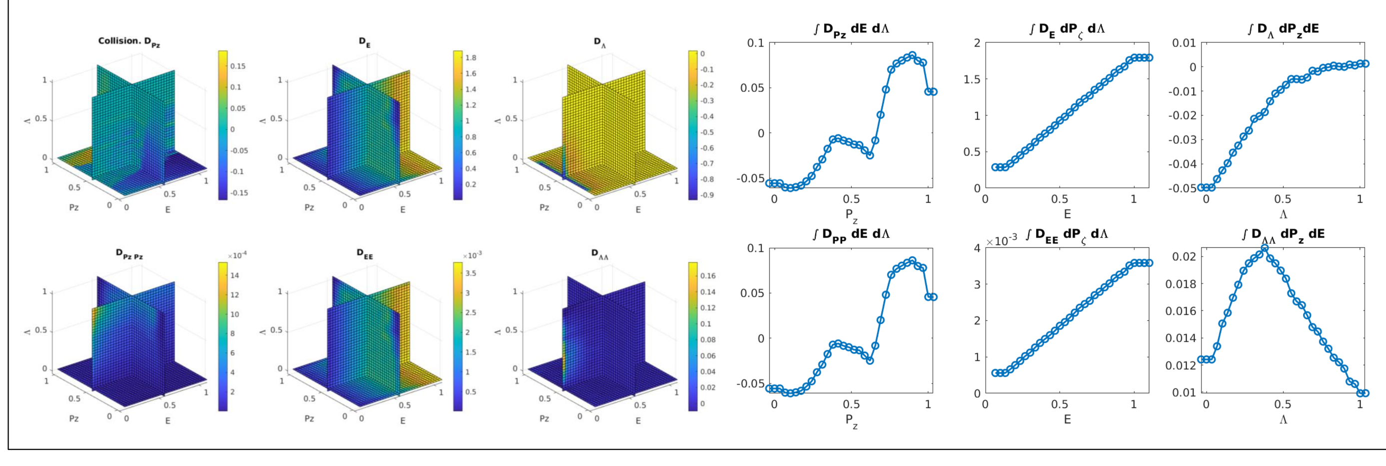
- **Averaged** D_{P_Z} **in the CoM space**
  - Co-passing particles: $D_{P_\zeta} > 0$, velocity drag; D_{P_Z} is larger since $v_{s\parallel}$ is related to $v_\parallel$; For trapped particles: $v_{s\parallel}$ is small
- **Compared with PSZS (resonant structures, localized), collision coefficients are global and related to particle orbit types.**
- Data size $(N_{P_\zeta}, N_E, N_\Lambda) = (128 \times 40 \times 20)$, stored in IDS. Raw data is interpolated and smoothed in the ATEP code to get the smooth function in the uniform grids in the CoM space.

D_{P_Z} Arbitrary units



Collision in the CoM space (ITER IMAS 100015/1)

- The simulation regime of energy is 100 KeV to 1 MeV. The energy is normalized to 1 MeV. The time unit is SI second. The normalization is chosen so that the normalized P_ζ and Λ are from 0 to 1. The collision coefficients are normalized accordingly.
- Background density and temperature are assumed to be uniform.
- Why choose $(E, \mu; \mu B < E$? The distribution functions will be almost half empty if using $E, \mu; \mu B < E$



- 1D integrated normalized collision coefficients
- $D_{\Lambda\Lambda} = 0$ at the $\Lambda = 0$ boundaries, Péclet number infinite→ the value of the $D_{\Lambda\Lambda}$ at the boundary is made equal to the values at two interior points

Implementation of the ATEP-3D

- **Discretization of the transport Eq. of EP**
  - Finite Volume Method (FVM): good conservation property
  - Fully implicit scheme (Crank-Nicholson): long time behavior
- **1D, 2D, 3D solver are developed using MATLAB; Fortran version planed.** 1D and 2D are used for fast testing, the conservation property, steady state studies
- **ATEP-3D: object oriented programming;** *atep3d*: core solver; *dist_exp_3d_cls*: experimental data interface

Discretization of the Eq. Using Uniform Grids and a fixed time step size.

The simulation domain is divided into $N_1 \times N_2 \times N_3$ cells with center values denoted using integer indices (i, j, k). ---- (P_ζ, E, Λ). Indices with half integers denotes the points on the cell faces, e.g. $(i \pm \frac{1}{2}, j, k)$

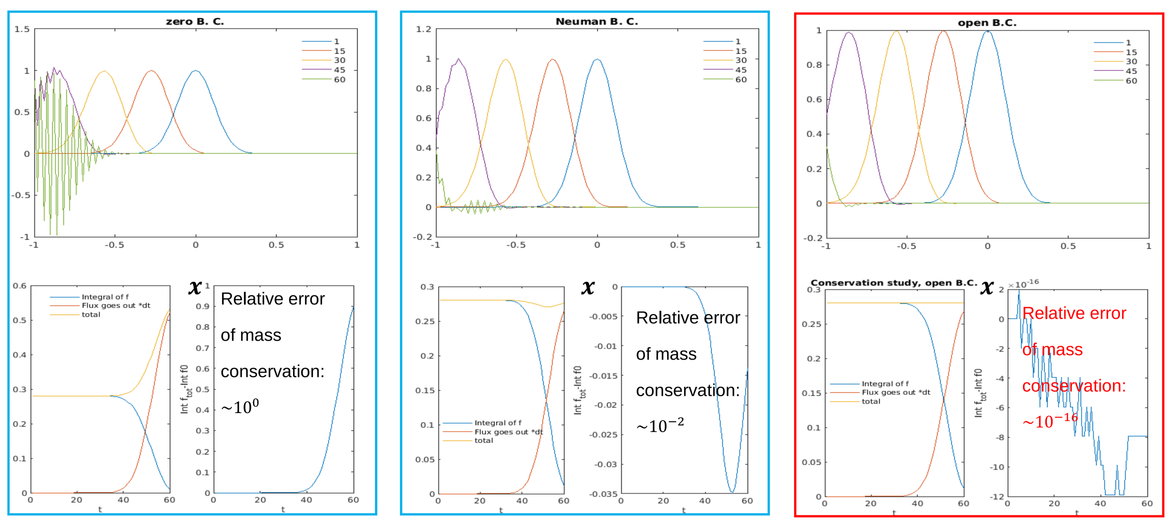
- Discretization of phase-space derivatives: linear centered scheme $f_{i\pm\frac{1}{2}} = \frac{1}{2}(f_i + f_{i\pm1})$
- Transport coefficients are dependent on phase-space coordinates but don't vary with time
- Boundary conditions are treated using a differential method

- Implicit Crank-Nicolson scheme for $\frac{\partial f}{\partial t} = C(f) + S$; C: collision; S: source
  $\frac{f^{l+1} - f^l}{\Delta t} = C\left(\frac{f^{l+1} + f^l}{2}\right) + S\left(\frac{f^{l+1} + f^l}{2}\right)$, Simplification: $S\left(\frac{f^{l+1} + f^l}{2}\right) \approx S(f^l)$, explicit source. l: time step index.
- One step in Matrix representation: $\bar{\bar{M}}^*_{LHS} \cdot \bar{F}^{l+1} = \bar{\bar{M}}^*_{RHS} \cdot \bar{F}^l + \bar{S}^l$
  - $\bar{\bar{M}}^*$ differential operator matrix, $\bar{F}^l$ and $\bar{S}$ are arrays of the distribution function f and the source function S. $f_{ijk} = \bar{F}_{i+(j-1)N_i+(k-1)N_iN_j}$. Note $\bar{\bar{M}}^*$ are constructed with chosen boundary conditions and is time-independent

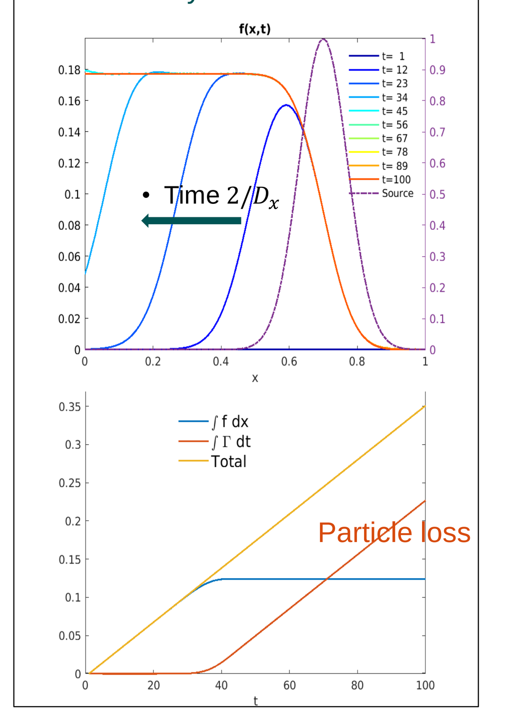
- **The advection terms (e.g., slowing down of energy due to collision) induce the shift of the distribution function** f **while the shape is preserved.** Negative flow: $\boldsymbol{D^\alpha > 0}$ (drag)
- The EPs are slowed down by the background and get lost at the boundaries. An open boundary condition is implemented that allows the flux to pass through the boundary without distorting the distribution function and without affecting the interior solution. **We propose open B.C:** $\frac{\partial^2 f}{\partial x^2} = 0$

1D conservation studies with different boundary conditions

- Test case: $\frac{\partial f}{\partial t} = D_x \frac{\partial f}{\partial x}$ $\quad D_x = 1,\quad f_0 = \exp(-x^2/0.025)$
- Analytical solution $f = \exp -(x + D_x t)^2/0.025$
- Numerical results: the particle number is conserved to machine precision by applying the open B.C.

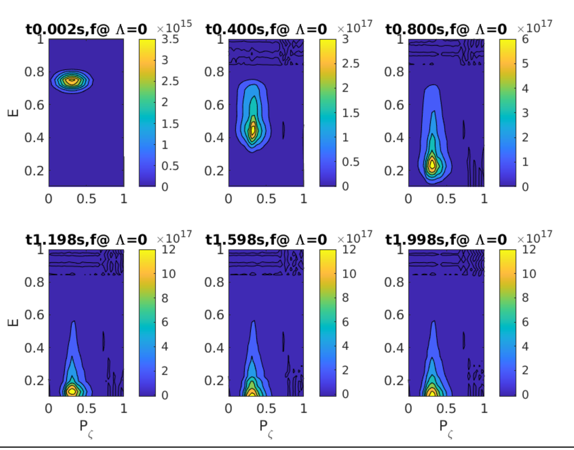


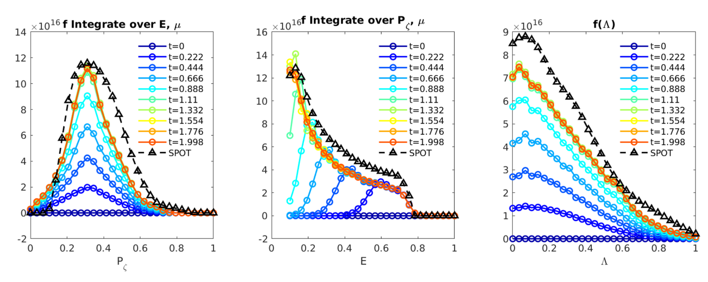
- Good conservation achieved in 1D Steady state studies



Steady state solution obtained with collision & source

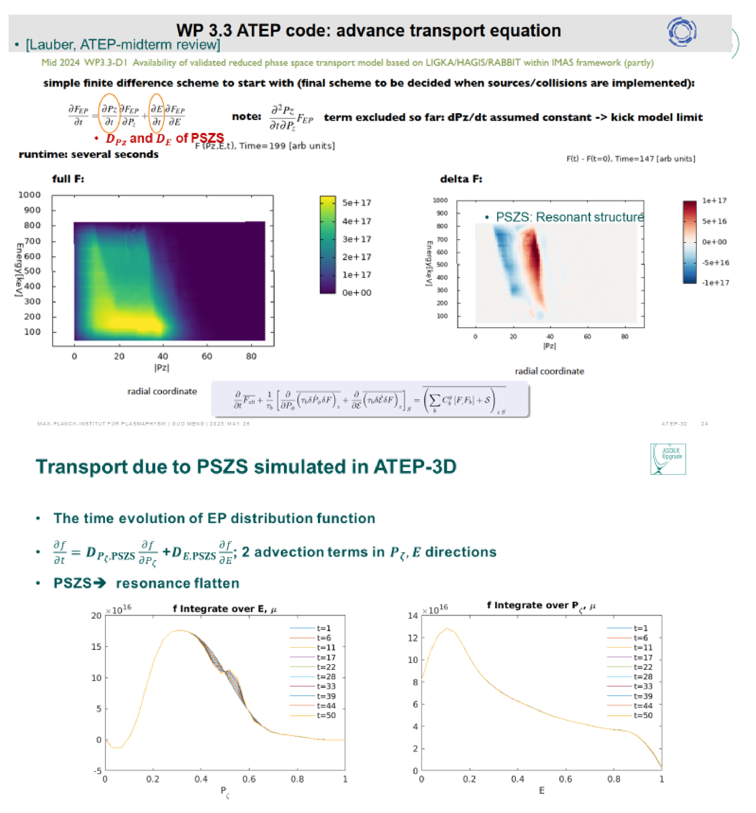
- **The slowing-down process of NBI induced EPs are simulated by ATEP-3D**
- **Source model: Gaussian function**
- $\boldsymbol{S = A_s \exp\left\{-\left[(P_\zeta - 0.31)^2/\delta P^2 + (E - 0.745)^2/\delta E^2 + (\Lambda - 0.1)^2/\delta\Lambda^2\right]\right\}}$





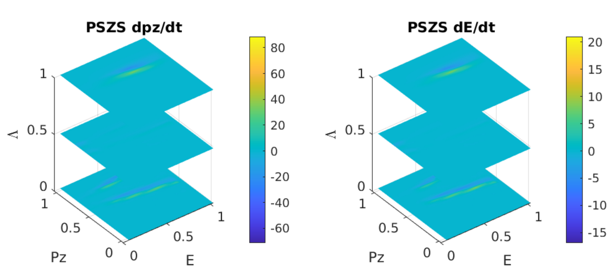
- **Comparison with SPOT**
- **Benchmark with other transport codes (TRANSP, ASCOT) is ongoing**

EP transport due to wave induced PSZS



PSZS induced by AEs

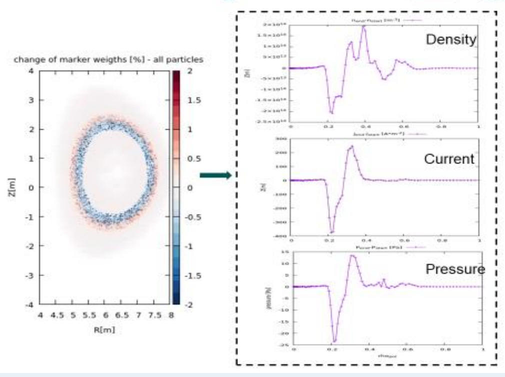
- $\frac{\partial f}{\partial t} = \frac{dP_Z}{dt}\frac{\partial f}{\partial P_Z} + \frac{dE}{dt}\frac{\partial f}{\partial E}$, introduce two advection terms of PSZS in P_Z and E directions



- In the kick model limit, a time-independent kick of the particle is assumed, indicated by $\frac{dP_z}{dt}$ and $\frac{dE}{dt}$ in the equation
- D_{P_Z} of PSZS is ~100 times of that due to collision
- D_E is ~10 times of that due to collision
- Larger at $\Lambda = 0$ and 1
- The PSZSs of EP have resonant structures and are very localized

Mapping between marker space and ATEP COM grids is produced *[6]*

- **Back-mapping to real space [Ph. Lauber]**
  - The 2D plot shows that the transport is indeed zonal by construction
- **Mapping to 1D profiles: density, current, pressure**
  - Parallel current is mainly peaked around the circulating particle transport region, whereas density and pressure are also affected by trapped particles (broader 1D profiles)



Summary and outlook

- Summary
  - ATEP-3D has been constructed fully embedded in the IMAS framework.
  - Code is setup in CoM space to describe accurately the evolution of PSZSs.
  - EP collision in CoM space is studied, instead of local pitch angle formulation.
  - Long time behavior of EP transport can be studied.
    - Steady state solution of EP slow-down using experimental data is simulated.
  - Mapping between marker space and ATEP CoM grids is produced→ density, current, pressure profiles.
- Outlook
  - Nonlinear PSZS measured by other gyrokinetic codes such as ORB5, TRIMEG.
  - Energy balance, EP distribution→ AE, zonal field evolution. Based on Zonca & Falessi model.
  - More physics ingredients (anomalous transport due to turbulence) can be included in the ATEP-3D. The transport coefficients in the CoM can be evaluated from simulations or theoretical models.
  - Add experimental source function in the CoM (RABBIT, IMAS).

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