Kinetic Model of Plasmas and Neutral Particles for Fusion Applications [1]

Oleg V. Batishchev

MIT PSFC, Cambridge, MA 02139, USA;
Lodestar Research Corporation, Boulder, CO 80301, USA;
Keldysh Institute, Moscow 125047, Russia

Motivation

The main reasons for the coupled plasma-neutrals kinetic modeling are coming from the tokamak scrape-off layer plasmas features and can be summarized as follows (the same arguments are applicable to ICF as well)

1. Finite (order of 0.1) ratios of electron and ion Coulomb m.f.p. to the connection lengths. It is known this is not small enough [1]. Thus the fluid description fails.
2. Sheath potential and particle/energy fluxes on the divertor strongly depend on the details of the plasma distributions.
3. The heat flux parallel to the magnetic field is carried mostly by the suprathermal electrons. Flux-limiting of the classical Spitzer-Harm result [2] at the midplane must be obtained self-consistently.
4. Electron-ion energy exchange time is bigger than the suprathermal electron bounce time.
5. Rates of electron-neutral interaction in the divertor are determined by the tail of the electron distribution function.
6. Knudsen number for neutral-neutral collisions can be high. The MC scheme is usually applied to treat them. Because of intrinsic noise, the fluid-MC hybrid codes can't find strictly converged solution.
7. Kinetic results are used to (i) verify fluid and hybrid plasma simulations, and (ii) to provide kinetic corrections.

These points have driven the new developments of Fokker-Planck code ALLA [3-5], listed below.

Set of equations. The plasma-neutrals mixture is described by a set of 3 non-linear kinetic equations (which are strongly coupled via collisions, electric field, and boundary conditions) for distribution functions $f_\alpha(t,x,v,\mu)$ (here $\alpha = e,i,N$; $\mu = v_{||}/v$, $v = \sqrt{v_{||}^2 + v_\perp^2}$, x and $v_{||}$ - are parallel to the magnetic line)

$$\frac{\partial f_e}{\partial t} + v\mu\frac{\partial f_e}{\partial x} - \frac{eE_x}{m_e}\frac{\partial f_e}{\partial v_x} = C_{ee} + C_{ei} + C_{EX} + C_I + S_e$$

$$\frac{\partial f_i}{\partial t} + v\mu\frac{\partial f_i}{\partial x} + \frac{eE_x}{m_i}\frac{\partial f_i}{\partial v_x} = C_{ii} + C_{CX} + S_i$$

$$\frac{\partial f_N}{\partial t} + v\mu\frac{\partial f_N}{\partial x} = C_{NN} + C_I + C_{CX} + S_N$$

where C_{ee}, C_{ei}, C_{ii} - Coulomb collisions terms, C_{EX}, C_I - N-excitation and ionization terms, C_{CX} - i-N charge exchange term, C_{NN} - neutral-neutral elastic collisions term, and S_α are boundary and volumetric mass/energy sources, respectively.

Challenges. Most severe difficulties of the electron-ion and plasma-neutral coupling arise from the intrinsic "stiffness" of the system, in particular:

- Different time scales must be resolved. These include the smallest e-e Coulomb time in the cold region, as well ion-ion characteristic time in the hottest region, and ion bounce time. Roughly time scale is varying from one hundredth of a microsecond to few milliseconds.

[1] Work supported by US DOE Grants No. DE-FG02-97-ER-54392 at Lodestar and DE-FG02-91-ER-54109 at MIT

- Collisionality is strongly varying across the SOL. Same species might be in different regimes (e.g. (1) tail electrons in the upstream region are collisionless, while thermal electrons near the edge are very collisional; (2) neutral transport might vary from the Navier-Stockes regime in the divertor to the Knudsen regime elsewhere.

- Different spatial scales also must be resolved. In the divertor, m.f.p. for plasma-plasma and plasma-neutrals and plasma parameters gradient lengths might be about centimeter, while the chamber dimensions are several meters.

- Different scales in the velocity space occur. We have to resolve sub-thermal ($T < 0.3eV$) ions and neutrals in the divertor, and supra-thermal electrons ($T > 300eV$) at the midplane.

Desired Properties (Physics). There are certain physical features of the plasma-neutrals system which have to be included in the coupled kinetic model:

- Local conservation laws (mass, momentum, energy balance);

- Global conservation of mass and energy (e.g. for the 100% recycling neutrals);

- In the 0-D treatment, plasma species and neutrals must self-equilibrate in the absence of unlike particles collisions, and mutually equilibrate in the presence of cross-species elastic collisions. The final distribution must be Maxwellian in all cases up to energies equal 100 kT;

- Smooth transition from low to high collisional regimes and back, giving the correct asymptotic behavior in both limits .

Desired Properties (Numerics). From the numerical point of view we want the method to be:

- Unconditionally stable (any time step), and conservative (fully, where applicable);

- Resolve sharp fronts, and allow wide range of the collisionality variation;

- Higher than first order accurate, and reasonably fast (100 h CPU on a desktop PC).

Numerical Model and Method Details

Non-uniform Adaptive Grid and Free-Streaming Term. The key element in our approach is the mesh used. In space it is 1D non-uniform and adaptive. The adoption scheme of a discrete function $\{f_i\}, i = \overline{0,N}, N \gg 1$ defined on a variable grid $\{x_i\}$ ($x \in [0, L]$) consist of the following steps [3]: (1) find cubic spline $F_3(x)$; (2) find function $G_3(x) = \int_0^x \mid \frac{dF_3}{dy} \mid dy$; (3) define $\Delta_x = (G_3(L) - F_3(0))/N$; (4) find $s_i = G_3^{-1}(i * \Delta_x), \ \overline{i = 1, N-1}$; (5) adjust (iteratively) new grid s_i to match two important constraints:

(i) $\delta_i \equiv s_{i+1} - s_i < S_x \gg \Delta_x/N$; (ii) $a^{-1} < \delta_{i+1}/\delta_i < a$, where $0 \leq a - 1 \leq 1$;

(6) calculate $g_i \equiv F_3(s_i)$; (7) finally multiply g_i by $\int f_i dx / \int g_i dx$ to get "mass" conservation, where $\int$ is the chosen numerical integration scheme (we used trapezoidal). This method was applied to the free-streaming equation which has a propagating solution:

$$\frac{\partial f}{\partial t} + v_{||} \ \frac{\partial f}{\partial x} = 0 \qquad \rightarrow \qquad f(t,x) = f(0, x - v_{||}t)$$

Test problem's simulation (propagation of two very narrow bell-shaped functions across the simulation domain) showed excellent results which were discussed in [6]. The velocity v, μ mesh is spherical axisymmetric (may be seen in Figs.3-4). The unknowns are cell-centered. The cell center coordinates are: $v_1 > 0$, $\Delta v_i \equiv v_{i+1} - v_i = c\Delta v_{i-1}, i > 2, \ c \geq 1$. Angular μ-grid is non-uniform, though it corresponds to a uniform azimuthal mesh. Cell's boundaries are picked in the way to give second order accurate evaluation of collisional fluxes. This combination allows (i) to treat cold ions and hot electrons on the same grid, (ii) to avoid singularity at the $v = 0$ axis, and (iii) allows easy parallelization on MPP [7].

Splitting with Adaptive Time Step. Second key moment is the usage of a time splitting scheme, with an adaptive sub-division of a fractional time step. For instance, for Coulomb collisions the sub-step is chosen locally, depending on the actual spatially evolving collisionality $\nu \propto n(t,x)/T^{1.5}(t,x)$.

The Coulomb term is

$$C_{\alpha/\beta} = \frac{L^{\alpha/\beta}}{v^2}\{ \quad \frac{\partial}{\partial v} v^2 [\frac{m_\alpha}{m_\beta}\frac{\partial \varphi^\beta}{\partial v} f^\alpha - \frac{\partial^2 \psi^\beta}{\partial v^2}\frac{\partial f^\alpha}{\partial v} - \frac{1-\mu^2}{v^2}(\frac{\partial^2 \psi^\beta}{\partial v \partial \mu} - \frac{1}{v}\frac{\partial \psi^\beta}{\partial \mu})\frac{\partial f^\alpha}{\partial \mu}] \; +$$
$$\frac{\partial}{\partial \mu}(1-\mu^2)[\frac{m_\alpha}{m_\beta}\frac{\partial \varphi^\beta}{\partial \mu} f^\alpha - (\frac{\partial^2 \psi^\beta}{\partial v \partial \mu} - \frac{1}{v}\frac{\partial \psi^\beta}{\partial \mu})\frac{\partial f^\alpha}{\partial v} - (\frac{1}{v}\frac{\partial \psi^\beta}{\partial v} + \frac{1-\mu^2}{v^2}\frac{\partial^2 \psi^\beta}{\partial \mu^2} - \frac{\mu}{v^2}\frac{\partial \psi^\beta}{\partial \mu})\frac{\partial f^\alpha}{\partial \mu}]$$

Here, Rosenbluth potentials $\varphi^\beta, \psi^\beta$ are obtained from coupled Poisson Equations:

$$\nabla^2 \varphi^\beta = f^\beta \quad , \quad \nabla^2 \psi^\beta = \varphi^\beta$$

which is discretized using 2nd order scheme. We must have $\delta\varphi/\varphi = 10^{-6}$ to get $\delta\psi/\psi = 10^{-3}$, which requires $v \times \mu = 200 \times 100$ mesh. Needed 9 derivatives are calculated using 3rd order differencing. FP coefficients are modified to give exactly Maxwellian tail in the 0-D steady-state.

Hydrogenic ion excitation (EX) and ionization (I) terms are

$$C_{EX} + C_I \;\; = \;\; N(t,x) \times \{ \sum_{p=I,EX} v\{-\sigma_p(v) f_e(v_{||}, v_\perp) + \sigma_p(a_p v) a_p^3 f_e(a_p v_{||}, a_p v_\perp) \; \} + \frac{\delta(v)}{2\pi v^2} K_I n_e \}$$

where σ_p, E_p = cross-sections, energy thresholds; $a_p = \sqrt{1 + 2E_p/(m_e v^2)}$; $K_I = \int \sigma_I v f_e d\vec{v}/n_e$ = ionization rate; $N(t,x)$=neutral density. Numerical scheme provides particle conservation: n_e for EX and $(n_i + n_e)$ for I; neutral distribution function remains non-negative, number of operation $\propto$ number of (v, μ) cells.

Hydrogen ion-neutral charge-exchange (CX) term is

$$C_{CX} \;\; = \;\; \sigma_{CX} \times \int \mid \vec{v} - \vec{u} \mid \{ f_n(\vec{v}) f_i(\vec{u}) - f_i(\vec{v}) f_n(\vec{u}) \} d\vec{u}$$

where σ_{CX} = constant cross-section. Numerical scheme is characterized by $n_i + n_N$ conservation (automatically momentum and energy); distribution functions remains non-negative, scheme takes into account the fact that f_α is 2V; total number of operation $\propto$ (number of (v, μ) cells)^2

Neutral collisions (NN) term. Most accurate description is given by the Boltzmann operator. However, since for the used (v, μ) grids total number of nodes is about 10K, and the CPU time would be unacceptable, we employ a simplified BGK approximation:

$$C_{NN} \;\; = \;\; \nu_{NN} \;\; (F_M - f_N)$$

where F_M is a drifted Maxwellian; ν_{NN} is the N-N collisional frequency. Used numerical scheme gives: conservation of mass, momentum and energy; non-negative distribution function; extremely fast performance.

Model problem. 2V two-species (four temperatures) plasma equilibration.

- Both electron and ion initial distribution are strongly non-Maxwellian, and all four initial temperatures are different: $T^i_\perp > T^i_{||} > T^e_\perp > T^e_{||}$;
- $M_i/m_e = 1836$ (the real value for hydrogen ions), and adaptive time step with 10^4 rise was used;
- Total 100 time steps took 200s run time on a PC, while conservation of mass, momentum and energy to - 10^{-8} (see Fig.1).

Realistic problem. 1D2V three-component system: electrons plus deuterium ions and atoms.

- C-Mod tokamak parameters: connection length - 10 m; line averaged density - 8 x 10^{19} m^{-3};
- Heating term (energy deposited into $T_\perp$) with 30 MWt/m^2 power is added into kinetic equation;
- 100% neutrals recycling at the divertor, and real mass ratio were adopted; BC similar to [8];
- Total physical time 10 microseconds; calculations took 6 CPU hours on a single processor PII/266.

Stationary profiles of e and i temperatures are shown in Fig.2. As can be seen (i) plasma species are not thermally equilibrated, and (ii) ion $T_{||}$ and $T_{\perp}$ are different. Figs.3 and 4 illustrate strongly non-Maxwellian particle distributions which were observed in our kinetic modeling for both plasmas and neutrals.

Conclusion

i First non-Monte-Carlo kinetic model for collisionally coupled electrons, ions and neutrals is developed.

ii The model includes some of the most important collisional processes in the SOL plasmas: plasma Coulomb and elastic neutral-neutral, hydrogen atoms impact ionization and excitation, hydrogenic ion-neutral charge-exchange. Addition of others (like three-body recombination) is straight forward.

iii The modified ALLA code can study both SOL plasma and neutral kinetics in 1D2V approximation for the realistic conditions of tokamaks and other fusion devices. The code 2D2V expansion is underway.

References [1] S.I.Krasheninnikov, *Contrib. Plasma Phys.* **34**, 151 (1994); [2] L.Spitzer and R.Harm, *Phys. Rev.* **89**, 977 (1953); [3] A.A.Batishcheva et al., Report PFC MIT, PFC/JA-95-23, August 1995; [4] A.A.Batishcheva et al., *Physics of Plasmas* **3**, 1634 (1996); [5] O.V.Batishchev et al., *Physics of Plasmas* **4**, 1672 (1997); [6] O.Batishchev et al., *Contrib. Plas. Phys.*, in print (1998); [7] A.A.Batishcheva et al., *Contrib. Plasma Phys.* **36** (2/3) 414 (1996); [8] R.J.Procassini et al., *Nucl. Fusion* **30**, 2329 (1990).

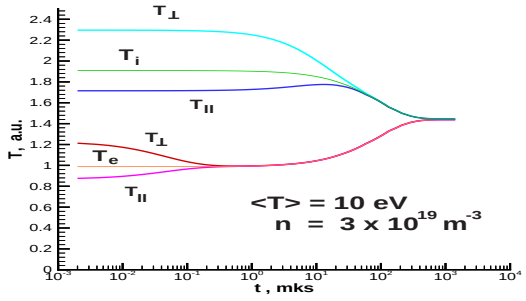

Fig.1.Four temperature equilibration

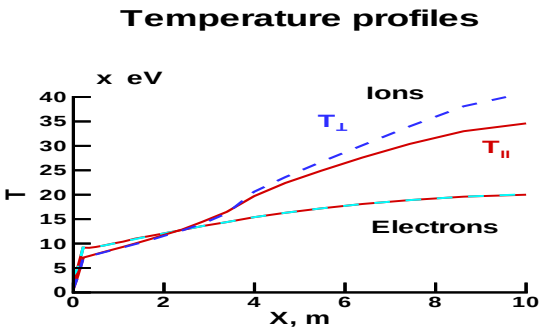

Fig.2.Electron and ion temperatures

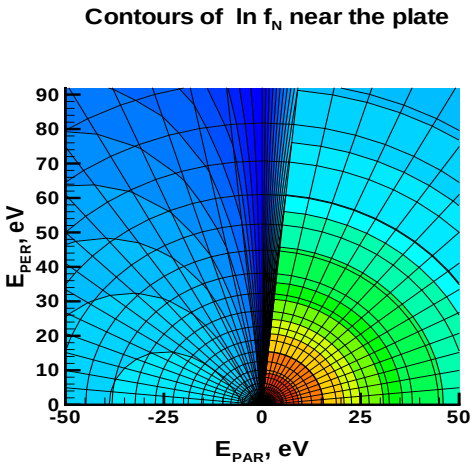

Fig.3.Neutrals distribution at the plate

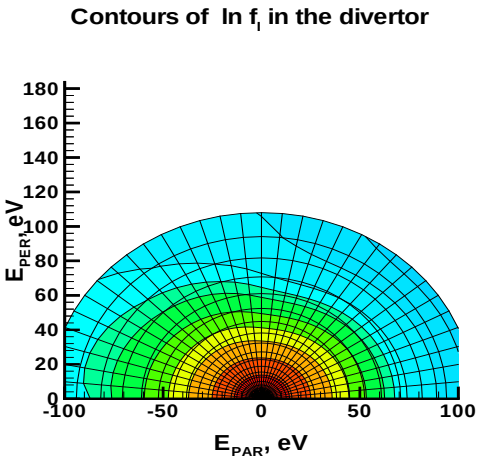

Fig.4.Ion distribution in the divertor

Author's e-mail, phone: oleg@psfc.mit.edu, (617) 253-5799