Notes on Collisions in GS2

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1 Existing electron collision operator in GS2

For a species "a" colliding with a Maxwellian species "b", the collision operator on f_a can be factored into two parts, a pitch-angle scattering operator and an energy diffusion and slowing down operator. Often one looks at just the pitch-angle scattering operator, since that is the dominant contribution to neoclassical transport and to collisional effects on trapped-particle instabilities (though for other problems the energy scattering is just as important as the pitch-angle scattering, even indirectly through energy scattering to lower energy where the pitch-angle scattering rate is larger).

GS2 also has options to try a Krook model collision operator, but here we will focus on the pitch-angle scattering operator, which can be written as:

$$\begin{aligned} df_a/dt &= C(f_a) \\ &= \sum_b C_{ab}(f_a) \\ &= \sum_b \nu_{\perp ab} \frac{1}{4} \frac{\partial}{\partial \xi} \left[(1-\xi^2) \frac{\partial f_a}{\partial \xi} \right] \end{aligned}$$

where $\xi = v_\parallel / v$ is the pitch angle. The pitch-angle scattering rate $\nu_{\perp ab}$ is given in the NRL formulary, p.31.

For electrons scattering off of other electrons and off of slow ions, this can be simplified to the form:

$$C(f_e) = \nu_e(E) \frac{1}{2} \frac{\partial}{\partial \xi} \left[(1-\xi^2) \frac{\partial f_e}{\partial \xi} \right]$$

(Note that this corrects a typo in Eq. 3 of KRT, where the factor of 1/2 was missing. This error exists only in the paper, not in the code.) $\nu_e(E)$, as given after Eq. 3 of Kotschenreuther, Rewoldt, Tang (Comp. Phys. Comm. **88**, 128 (1995)), is

$$\nu_e(E) = \nu_{ei} \left(\frac{v_{2e}}{v} \right)^3 [Z_{eff} + H_{ee}(v/v_{2e})]$$

with $v_{2e} \equiv (2T_e/m_e)^{1/2}$, and $\nu_{ei} \equiv 4\pi n_e e^4 \log \lambda / [(2T_e)^{3/2} m_e^{1/2}]$. This is the operator used for electron collisions in GS2, and its usage can be seen in `collisions.f90`.

The GS2 input parameter `vnewk` is the value of ν_{ei} normalized by $a/(v_t\sqrt{2})$, where $v_t \equiv \sqrt{T_{ref}/m_{ref}}$. [This is related to the time step used internally in the code. For example, when `wstar_units=.false.`, the time step is $\Delta t = (\texttt{delt}) \times a/v_t/\sqrt{2}$, where `delt` is a namelist input parameter.] Thus `vnewk` for electrons is:

$$\texttt{vnewk}_e = \nu_{ei}\frac{a}{\sqrt{2}v_t} = \frac{4\pi n_e e^4 \log\Lambda}{(2T_e)^{3/2} m_e^{1/2}}\frac{a}{\sqrt{2}v_t} = 0.002791\frac{n_{e19}\log\Lambda}{T_{e,keV}^{3/2}}\frac{a_m A_{ref}^{1/2}}{T_{ref,keV}^{1/2}}$$

where density n_{e19} is in units of $10^{19}/m^3$, the electron temperature $T_{e,keV}$ is in keV, the normalizing macroscale a_m is in meters, and the reference specie used for normalizing has temperature $T_{ref,keV}$ in keV, and atomic mass (relative to the proton) of A_{ref}. (Some of the earlier documentation for the GS2 namelist had a definition of `vnewk` that was hardwired to $A_{ref} = 2$, but the above formula allows it to be scaled to any A_{ref}.)

2 Ion collision operator in GS2

For ions scattering off of other ions of the same species, we get a related form:

$$C(f_i) = \nu_{ii}(E)\frac{1}{2}\frac{\partial}{\partial\xi}\left[(1-\xi^2)\frac{\partial f_i}{\partial\xi}\right]$$

with

$$\nu_{ii}(E) = \nu_{ii}\left(\frac{v_{2i}}{v}\right)^3 H_{ee}(v/v_{2i})$$

At present, GS2 only includes collisions of an ion species with itself, so the ion collision operator is of this form. The `vnewk` parameter for the ions is the normalized $\nu_{ii}a/(v_t 2^{1/2})$, where ν_{ii} is like ν_{ei} but with electron quantities replaced by ion quantities.

To work this out a little more explicitly, assume the plasma has two main ion species, a lighter ion species (typically hydrogenic ions, but might be $Z = 2$ helium in some cases) with density, charge and mass n_i, Z_i and A_i, and a heavier ion species (typically carbon or other impurities) with n_I, Z_I, A_I. (We distinguish between light ions and heavy ions because of the difference in the collision operator between colliding with comparable mass particles and disparate mass particles, which shows up in the properties of the H_{ee} function at high and low relative velocities.) The densities are given by

$$\frac{n_i Z_i}{n_e} = \frac{Z_I - Z_{eff}}{Z_I - Z_i}$$
$$\frac{n_I Z_I}{n_e} = \frac{Z_{eff} - Z_i}{Z_I - Z_i} \quad (1)$$

For the lighter ion species, you can approximately include the effect of collisions on heavier impurities as well by enhancing the collision frequency by a factor of Z_{eff}

(similar to what is done for electron-ion collisions). Thus, the resulting value of the $\texttt{vnewk}_i$ parameter for the lighter ions can be related to the above value $\texttt{vnewk}_e$ for electrons by:

$$\texttt{vnewk}_i = \texttt{vnewk}_e \;\; Z_i^2 Z_{eff} \left(\frac{m_e}{m_i}\right)^{1/2} \left(\frac{T_e}{T_i}\right)^{3/2} \tag{2}$$

One could use a similar expression for beam species, and replace T_i with an average beam temperature.

For heavier impurities, the approximation that impurity-(light ion) collisions is negligible compare to impurity-impurity collisions is approximately that

$$\frac{\nu_\perp^{Ii}}{\nu_\perp^{II}} = \frac{A_i^{1/2} n_i Z_i^2}{A_I^{1/2} n_I Z_I^2} = \left(\frac{A_i}{A_I}\right)^{1/2} \left(\frac{Z_i}{Z_I}\right) \frac{Z_I - Z_{eff}}{Z_{eff} - Z_i} \ll 1 \tag{3}$$

This was derived by looking at the expressions on p.32 of the NRL for slow ions pitch-angle scattering off of other ions, and using Eq. (1) to relate n_i/n_e and n_I/n_e to Z_{eff}. If this is satisfied, then the GS2 input parameter for the impurities is

$$\texttt{vnewk}_I = \texttt{vnewk}_e \;\; \frac{n_I Z_I^4}{n_e} \left(\frac{m_e}{m_I}\right)^{1/2} \left(\frac{T_e}{T_I}\right)^{3/2}$$

To roughly account for pitch-angle scattering of heavy impurities by lighter species, we can add a term related to Eq. (3) to get

$$\texttt{vnewk}_I = \texttt{vnewk}_e \;\; \left(\frac{m_e}{m_I}\right)^{1/2} \left(\frac{T_e}{T_I}\right)^{3/2} \frac{Z_I^3}{Z_I - Z_i} \left[Z_{eff} - Z_i + \left(\frac{A_i}{A_I}\right)^{1/2} \frac{Z_i}{Z_I} (Z_I - Z_{eff}) \right]$$

And we see that this gives a finite collision frequency even in the limit $Z_{eff} \to Z_i$.

One can construct a Padé approximation that merges both the slow and fast ion limits into a single formula and so should be roughly okay for any ion species:

$$\texttt{vnewk}_i = \texttt{vnewk}_e \;\; \left(\frac{m_e}{m_i}\right)^{1/2} \left(\frac{T_e}{T_i}\right)^{3/2} Z_i^2 \sum_\beta \frac{n_\beta Z_\beta^2}{n_e} \frac{2}{1 + (A_i/A_\beta)^{1/2} (T_\beta/T_i)^{1/2}}$$

where $\sum_\beta$ is the sum over all species that species i is colliding with (including like-particle collisions with $\beta = i$). [This is probably a bit more accurate that Eq. (2), from which it differs a bit because of the limitations of using a single v_{2i} in the $H_{ee}(v/v_{2i})$ function to describe the velocity dependence of collisions with all other ion species. But it was constructed so that for like-particle collisions in the $Z_{eff} = Z_i$ limit it reproduces Eq. (2) exactly.]

3 Momentum conserving term

For ion-ion collisions, GS2 includes a momentum restoring term (if the namelist option `conserve_momentum=.true.`):

$$\frac{\partial f_i}{\partial t} = \nu_{ii}(E) \frac{1}{2} \frac{\partial}{\partial \xi} \left[(1 - \xi^2) \frac{\partial f_i}{\partial \xi} \right] + S(E)\xi$$

where $S(E)$ is chosen after each time step to conserve the momentum within a species at a given energy integrated over all pitch angles. I.e. $\int d\xi f_i(E,\xi)\xi$ is conserved. This is somewhat different from other formulations, where it is only the momentum integrated over all pitch-angles and energies that is conserved, and the momentum restoring term is a Maxwellian times ξ. Bill Dorland recalls discussions on this issue with Kotschenreuther, and says that there is some discussion of this issue near the end of Hinton and Hazeltine's Rev. of Modern Physics neoclassical article, where they reference some Russian paper that shows that this allows the use of a variational principle used in certain analytic results, so that the code can be checked exactly against those analytic results.

Momentum is not conserved for electron collisions in GS2, as is appropriate for electron-ion collisions (this neglects the electron-electron part which would conserve collisions). In most cases, one would choose `conserve_momentum=.true.`, and this is probably important for neoclassical damping of poloidal flow in nonlinear runs. In reality however, hydrogenic ions can exchange momentum with impurities via collisions. In some cases, this might have an effect on growth rates of instabilities, since the resonance conditions for hydrogenic and impurity species are different. The current/momentum ratio may also differ between species (perhaps more so if there is a significant amount of tritium compared to other species with a charge to mass ratio of 1/2).

4 Possible upgrades to the collision operator in GS2

As described above, GS2 at present has the pitch-angle scattering operator, and only for collisions of one species with itself (except for electrons, where electron-ion collisions are included). Using the above approximations, one can approximately include the effect of collisions with other species. I believe it should be possible to eventually upgrade the collision operator in GS2 to better handle collisions between species, momentum-exchange between species, and even include energy scattering and slowing-down. But for now this is a good first cut, and the parameters and approximations are documented here.