Development of Coulomb collision operator for multiple-ion-species neoclassical transport simulation

多イオン種新古典輸送シミュレーションに向けたクーロン衝突項の開発

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To study and evaluate the neoclassical transport process in burning plasma in nuclear fusion reactor, it is required to develop a neoclassical transport simulation code for multiple ion species plasma which treats the Coulomb collisions between unlike ion species. We extend the global neoclassical simulation code FORTEC-3D by implementing the unlike-species collision operator which keeps the self-adjointness nature even if the temperature of two ion species are different (Sugama et al., Phys. Plasmas **16** (2009) 112503). In this paper, a numerical method to implement the collision operator in the δf PIC drift-kinetic code is explained. Also, a possible numerical technique to reduce the computation time of multiple-ion-species collision operator is discussed.

1. Introduction

In research toward the realization of nuclear fusion reactor, numerical simulation which enables us to reproduce and expect the transport process in burning plasma is required. One of the important differences between the burning plasma from that in the present plasma confinement experiments is that the former necessarily consists of multiple ion species such as D, T as well as He ash and impurities from the wall. Ion mass-ratio and isotope effects are of importance to control D-T reactor.

Collision operator for unlike-species in drift-kinetic and gyrokinetic simulations are required to simulate neoclassical and micro-scale turbulent transports. In plasma kinetic theory and simulation, it is conventionally assumed that all ion species have the same temperature. The linearized Landau operator for unlike-species collision [1] satisfies the self-adjointness property only when two colliding ions have the same temperature, $T_a = T_b$. The adjointness of the operator is required to ensure the H-theorem and Onsager symmetry of the transport matrix of collisional transport, which are the important features to investigate a dissipative transport process. Sugama et al. has developed a modified linearized collision operator [2] which keeps the adjointness property even if $T_a \neq T_b$. As shown in [2], the part which breaks the adjointness in the original collision operator is proportional to $(1 - T_b/T_a)$. Therefore, application of the adjoint collision operator is important in the cases when the difference in ion temperatures is large.

2. Self-adjoint unlike-species collision operator

Linearized collision operator has the test-particle and field-particle parts as follows:
$$C_{ab}^L(\delta f_a, \delta f_b) = C_{ab}^T(\delta f_a) + C_{ab}^F(\delta f_b). \quad (1)$$
The self-adjoint test-particle operator is given by
$$C_{ab}^T(\delta f_a) = Q_{ab} C_{ab}^{T0} Q_{ab} \delta f_a, \quad (2)$$
where C_{ab}^{T0} is the pitch-angle and energy scattering operators, and $Q_{ab}g \equiv g + (\theta_{ab} - 1)P_a g$. P_a is defined in [2]. The parameter θ_{ab} is defined as
$$\theta_{ab} \equiv \sqrt{T_a \left(\frac{1}{m_a} + \frac{1}{m_b}\right) \Big/ \left(\frac{T_a}{m_a} + \frac{T_b}{m_b}\right)}, \quad (3)$$
which expresses the degree of modification of the linearized collision operator to keep the adjointness, and $\theta_{ab} - 1 = 0$ in the limit $T_a = T_b$. On the other hand, the field-particle operator is given by
$$C_{ab}^F(\delta f_b) = -V_{ab}[\delta f_b] \cdot C_{ab}^T(f_{aM} m_a v_{\parallel}/T_a)$$
$$- W_{ab}[\delta f_b] \cdot C_{ab}^T(f_{aM} x_a^2), \quad (4)$$
where $x_a^2 \equiv v^2/v_{ta}^2$, f_{aM} is the Maxwellian, and V_{ab} and W_{ab} are defined as
$$V_{ab}[\delta f_b] \equiv \frac{T_b}{\gamma_{ab}} \int d^3v \frac{\delta f_b}{f_{bM}} C_{ba}^T(f_{bM} m_b v_{\parallel}/T_b), \quad (5a)$$
$$W_{ab}[\delta f_b] \equiv \frac{T_b}{\eta_{ab}} \int d^3v \frac{\delta f_b}{f_{bM}} C_{ba}^T(f_{bM} x_b^2). \quad (5b)$$
Here, γ_{ab} and η_{ab} are related to collision frequency between *a* and *b* species. The modified collision operator is self-adjoint and also satisfies the conservation law of momentum and energy, which is another important property for linearized Landau operator. Simpler unlike-particle operator, for example the one in [3], only satisfies the conservation law, and self-adjointness is satisfied only if $T_a = T_b$.

3. Implementation of the collision operator in δf PIC neoclassical transport code

In a δf PIC code like FORTEC-3D[4], which already implements the adjoint and conserved collision operator for like-particle collisions, the test-particle operator C_{ab}^{T0} for unlike-particle collisions can be implemented in the same way as the like-particle one, by giving random walk to each simulation marker's velocity. Taking time integral of eq. (1) over a short time Δt, the change of δf_a at i-th marker position by test-particle operator is expressed as

$$\delta f_a(\boldsymbol{v}_i + \Delta \boldsymbol{v}_i; t + \Delta t)|_{C_{ab}^T} = \delta f_a(\boldsymbol{v}_i; t) +$$

$$S_{ab}^T(\Delta U_{ab}^{T0}, \Delta E_{ab}^{T0}, \boldsymbol{v}_i + \Delta \boldsymbol{v}_i) f_{aM}(\boldsymbol{v}_i + \Delta \boldsymbol{v}_i), \quad (6)$$

where $\boldsymbol{v}_i$ is the i-th marker velocity and $\Delta \boldsymbol{v}_i$ is the random walk by C_{ab}^{T0}, and S_{ab}^T corresponds to the $(\theta_{ab} - 1)P_a g$ part in Q_{ab}, which is functional of $\Delta U_{ab}^{T0} = \int d^3v\, v_\parallel [\delta f_a(\mathbf{v}, t + \Delta t) - \delta f_a(\mathbf{v}, t)]$ and $\Delta E_{ab}^{T0} = \int d^3v\, v^2 [\delta f_a(\mathbf{v}, t + \Delta t) - \delta f_a(\mathbf{v}, t)]$. Therefore, total C_{ab}^T can be implemented by the ordinal random walk part C_{ab}^{T0} and a source term S_{ab}^T, which is functional of momentum and energy change by the random walk, ΔU_{ab}^{T0} and ΔE_{ab}^{T0}.

Concerning the field-particle part, one needs to evaluate Eq. (5). However, using the self-adjointness of C_{ab}^T, we obtain

$$V_{ab}[\delta f_b] \equiv \frac{m_b}{\gamma_{ab}} \int d^3v\, v_\parallel C_{ba}^T(\delta f_b) = \frac{m_b}{\gamma_{ab}} \frac{\Delta U_{ba}^T}{\Delta t}, \quad (7a)$$

$$W_{ab}[\delta f_b] \equiv \frac{m_b}{2\eta_{ab}} \int d^3v\, v^2 C_{ba}^T(\delta f_b) = \frac{m_b}{\gamma_{ab}} \frac{\Delta E_{ba}^T}{\Delta t}, \quad (7b)$$

where ΔU_{ab}^T and ΔE_{ab}^T represent the momentum and energy change after C_{ba}^T is operated to δf_b, respectively. Eq. (7) is easier to evaluate in a PIC code than Eq. (5).

In reality, it is known that a direct numerical implementation of C_{ab}^T and C_{ab}^F by Eqs. (6) and (7) in a particle code inevitably breaks the conservation of total particle number, momentum, and energy, because of insufficient accuracy in taking velocity integrals. The accumulation of the numerical error and its propagation among particle species may cause a problem to achieve steady-state solution. To avoid the problem, multiple ion species FORTEC-3D will adopts the same method to ensure the conservation property as used in the single-species vesion[4], by modifying the form of Eq. (4) slightly.

One thing to be noted for the application of unlike-species collision operator is the importance of Coulomb logarithm appearing in the definition of collision frequencies, γ_{ab} and η_{ab}. Even if one uses an elaborate linearized collision operator, inadequate choice of the formula for $\ln\Lambda_{ab}$ may cause 10~20% difference. Recently, Honda[5] has derived a useful and reliable formula for $\ln\Lambda_{ab}$ with taking account of the temperature difference. FORTEC-3D will use the formula.

4. Reduction of communication time

Both C_{ab}^T and C_{ab}^F requires to take velocity moments of δf_a and δf_b. In running FORTEC-3D code on a supercomputer with many nodes, this procedure needs MPI_ALLGATHER reduction communication, which takes substantial time as the number of computation nodes increases. Therefore, some programming technique to reduce the communication time should be adopted.

The linearized collision term between a-b species is independent of another combination c-d. Therefore, there are several ways to reduce the actual consumption time for collision operator by overlapping the communication with calculation. One example is to overlap the computation of C_{ab}^{T0} and the moments $\Delta U(,E)_{ab}^{T0}$ on each MPI rank with the reduction of $\Delta U(,E)_{cd}^{T0}$ among the MPI ranks, including $\Delta U(,E)_{ba}^{T0}$. Another way is to overlap the calculation of $\Delta U(,E)_{ab}^T$ with the reduction of $\Delta U(,E)_{cd}^{T0}$. To hide collective communication like MPI_ALLGATHER to the background of computation time, we need a different method from the overlapping method of asynchronous communication like MPI_ISEND /_IRECV with computation. Using OpenMP thread-parallel, while one thread communicates with other MPI ranks, all the remaining thread are engaged in taking moments on each MPI rank. The basic idea for the overlapping method in MPI/OpenMP hybrid parallel computation was proposed by Maeyama et al.[6].

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