Development of a Lagrange-Monte-Carlo Scheme for Fluid Modeling of SOL/Divertor Plasmas

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Aiming at reproducing plasma detachment states with a three-dimensional fluid code, we are developing the Lagrange-Monte-Carlo scheme. It integrates two schemes, namely a Lagrange scheme for the convective part and a Monte-Carlo scheme for the diffusive part. One advantage of the scheme is the semi-implicit treatment of the pressure gradient term in the convective part, essential to solve pure-convective problems. As a first step, several one-dimensional (1D) test calculations have been done so far. In this paper, results of the two preliminary tests are presented; 1) a test for the Lagrange-scheme solving convective equations and 2) a test for the integrated Lagrange-Monte-Carlo scheme solving a convection-conduction equation. These tests confirm conservative property of the Lagrange scheme and reliability of the integrated Lagrange-Monte-Carlo scheme.

1. Introduction

For future fusion reactors, detachment is a necessary condition to keep the heat and the particle loads to the divertor plate in manageable levels. Therefore, to understand requirements for stable operation under detached conditions, several numerical codes exist like SOLPS[1][2], SONIC[3][4], and EMC3-EIRENE[5][6][7]. In contrast to 2D, it remains an issue to produce the detachment state with a three-dimensional plasma fluid code. That is not only for 3D stellarators. Even in Tokamaks, the axial symmetry does not hold due to the existence of some gas-pumping/puffing ports and other structures. In order to treat such asymmetric structures, a three-dimensional fluid code is surely required to get a predictable model of the detachment state for future fusion reactors.

One difficult matter for a plasma transport code is that there is a strong anisotropy of transport between (classical) parallel transport along magnetic field lines and (anomalous) radial transport. This produces numerical accuracy problems solving the discretization matrix equations for finite discretization methods, i.e., finite-difference, finite-volumes, and finite-elements. To avoid that, we started to develop a plasma fluid code with the Monte Carlo scheme (MC) which uses pseudo fluid-particles representing a certain amount of e.g., plasma density, momentum, internal energy. MC is based on a random walk approach derived for Fokker-Planck-like transport equations. Therefore, it is very well suited for solving diffusive problems. However, MC fails to obtain the right solution in some pure convective cases, probably linked to its explicit treatment of the pressure gradient term. To overcome this problem, we use the Lagrange scheme (LG), because it is easy for the LG to implement a semi-implicit treatment of the pressure gradient term.

Combining these two approaches, we developed a LG-MC scheme, which integrates the advantages of both schemes using LG for the convective and MC for the diffusive part. So far, we got one-dimensional coupled results of the continuity, momentum, and energy equations in a simple 1D model geometry along the field line.

In this paper, we present first results obtained by LG and LG-MC. The next section will focus on the detailed description of LG-MC. The 1D results will be shown in Sec. 3 and the summary will be given in Sec. 4.

2. The Lagrange-Monte-Carlo Scheme

As a 1D fluid model along the field line, we introduce the continuity, momentum, and energy equations as follows;

$$\frac{\partial n}{\partial t} + \frac{\partial}{\partial x}(nV) = S_n, \tag{1}$$

$$\frac{\partial}{\partial t}(mnV) + \frac{\partial}{\partial x}(mnV^2 + p) = S_V, p = n(T_i + T_e), \tag{2}$$

$$\frac{\partial}{\partial t}(\frac{3}{2}nT_i + \frac{1}{2}mnV^2) + \frac{\partial}{\partial x}(\frac{1}{2}mnV^3 + \frac{5}{2}nVT_i - \kappa_i\frac{\partial T_i}{\partial x}) = S_{T_i}, \tag{3}$$

$$\frac{\partial}{\partial t}(\frac{3}{2}nT_e) + \frac{\partial}{\partial x}(\frac{5}{2}nVT_e - \kappa_e\frac{\partial T_e}{\partial x}) = S_{T_e}, \tag{4}$$

where m is the ion mass, n, V, T_i, and T_e are the plasma density, the ion flow velocity, the ion temperature, and the electron temperature, respectively. The arc length, x, along the field line is used as the spatial coordinate. The symbols S_n, S_V, S_{T_i}, and S_{T_e} denote the source/sink terms of the particle, momentum, ion heat, and electron heat, respectively. In addition, parallel thermal conductivity of the ions and that of the electrons are represented by κ_i and κ_e. The ion energy equation, Eq.(3), is reformulated with Eqs.(1) and (2) as

$$\frac{\partial}{\partial t}(\frac{3}{2}nT_i) + \frac{\partial}{\partial x}(\frac{3}{2}nVT_i - \kappa\frac{\partial T_i}{\partial x}) + nT_i\frac{\partial V}{\partial x} = S_{T_i} + \frac{1}{2}mV^2S_n. \tag{5}$$

In LG-MC, Eqs.(1), (2), (4) and (5) are solved as a coupled problem. The algorithm of the scheme is divided into three sub-steps, i) Initialization of particles and Source, ii) Convection, and iii) Diffusion. For simplicity, in this section, the description of the algorithm will be given for a coupled problem of Eqs. (1),(2), and (5). Hereafter, the symbol T and S_T denote the ion temperature and the ion heat source term, respectively.

i) Initialization of particles and Source

First we introduce "Lagrange particles". The Lagrange particles have three kinds of weight, W_n for density n, W_V for the momentum mnV, and W_T for the internal energy $3nT/2$ so that they satisfy

$$n_j = \frac{N_jW_n}{\Delta V_j}, mn_jV_j = \frac{N_jW_V}{\Delta V_j}, \frac{3}{2}n_jT_j = \frac{N_jW_T}{\Delta V_j}. \tag{6}$$

where N_j is the number of the total Lagrange particles in the j-th cell and ΔV_j is the cell volume. It should be noted that W_n is a fixed value while W_V and W_T change during calculations. The way to update them will be described in the next section, ii) Convection sub-step. Thus, as the initial setting, N_j is determined by the initial density profile and the constant W_n, then N_j Lagrange particles having W_n are uniformly distributed in each cell. The other weights, W_V and W_T, are determined in each cell according to the initial velocity and temperature profiles.

For the source terms, new Lagrange particles are added to the calculation domain according to the source terms in Eqs.(1),(2), and (5). The number of the added particles N_{add} and their weights are determined in each cell as;

$$N_{add} = \frac{S_n\Delta t\Delta V}{W_n}, W_V = \frac{W_nS_V}{S_n}, W_T = \frac{W_n}{S_n}(S_T + \frac{1}{2}mV^2S_n). \tag{7}$$

where Δt is a discretized time step.

ii) Convection

We treat all the terms except for the diffusive terms and source terms in this sub-step. Equations (1),(2), and (5) are reformulated with Lagrange derivative, $\frac{d}{dt} \equiv \frac{\partial}{\partial t} + V\frac{\partial}{\partial x}$ as follows;

$$\frac{\partial n}{\partial t} + \frac{\partial nV}{\partial x} = 0 \longrightarrow \frac{dn}{dt} = -n\frac{\partial V}{\partial x}. \tag{8}$$

$$\frac{\partial}{\partial t}mnV + \frac{\partial}{\partial x}(mnV^2 + nT) = 0 \longrightarrow \frac{dV}{dt} = -\frac{1}{mn}\frac{\partial nT}{\partial x}. \tag{9}$$

$$\frac{\partial}{\partial t}(\frac{3}{2}nT) + \frac{\partial}{\partial x}(\frac{3}{2}nVT) + nT\frac{\partial V}{\partial x} = 0 \longrightarrow \frac{dT}{dt} = -\frac{2}{3}T\frac{\partial V}{\partial x}. \tag{10}$$

Now all the calculated values, n, V, and T, are on the Lagrangian coordinate. To calculate them numerically with the Lagrange particles, we first renew the weights W_V and W_T with Eqs.(9) and (10) as follows;

$$W_V^* = mW_nV^* = mW_n(V - \frac{1}{mn}\frac{\partial nT}{\partial x}\Delta t), \tag{11}$$

$$W_T^* = \frac{3}{2}W_nT^* = \frac{3}{2}W_n(T - \frac{2}{3}T\frac{\partial V}{\partial x}\Delta t). \tag{12}$$

Then the Lagrange particles having W_n, W_V^*, and W_T^* move with V_p as follows;

$$x(p)^{new} = x(p)^{old} + V_p\Delta t, \tag{13}$$

where $x(p)^{new(old)}$ is the new(old) position of the p-th Lagrange particle. V_p is obtained from interpolation of the renewed velocities V^* at the old position of the p-th particle. The use of V^* (not V) which is updated by the pressure gradient enables the semi-implicit treatment for the pressure gradient terms.

iii) Diffusion

Finally, the weight of the internal energy of the Lagrange particles are updated by the remaining term, the heat conduction term. This is done by a Monte-Carlo scheme[8], solving the following equation;

$$\frac{\partial}{\partial t}(\frac{3}{2}nT) + \frac{\partial}{\partial x}(-\kappa\frac{\partial T}{\partial x}) = 0. \tag{14}$$

At the beginning of this sub-step, "Monte-Carlo particles" are copied from the Lagrange particles, i.e., they take over the positions and the weights of the Lagrange particles. Different to the Lagrange particles, however, the Monte-Carlo particles have only one kind of weight, e.g., the internal energy $3nT/2$ for the energy equation. The same is possible for viscous conduction in the momentum equation. To apply MC, Eq. (14) is rewritten as a partial differential equation;

$$\frac{\partial}{\partial t}(\frac{3}{2}nT) + \frac{\partial}{\partial x}(-\frac{2\kappa}{3n}\frac{\partial}{\partial x}(\frac{3}{2}nT) - \frac{2\kappa}{3}(\frac{\partial}{\partial x}\frac{1}{n})\frac{3}{2}nT) = 0. \tag{15}$$

Using the two-step method[7], transport of the Monte-Carlo particles is implemented;

$$x_T(p)^i = x_T(p)^s + \sqrt{2\frac{2\kappa}{3n}(x^s)\delta t}\xi, \tag{16}$$

$$x_T(p)^f = x_T(p)^s + \sqrt{2\frac{2\kappa}{3n}(x^i)\delta t}\xi - \frac{2\kappa}{3}(\frac{\partial}{\partial x}\frac{1}{n})(x^s)\delta t, \tag{17}$$

where $x_T(p)^s$, $x_T(p)^i$, $x_T(p)^f$, and δt are starting position, intermediate position, final position of the p-th Monte-Carlo particle, and a discretized time step for this sub-step. The symbol ξ is a normal random number which satisfies $\langle\xi\rangle = 0$ and $\langle\xi^2\rangle = 1$. After this sub-step, we obtain new temperature profile from the distribution of the Monte-Carlo particles. Then the weight of the internal energy of the Lagrange particles are replaced by the new temperature. That is the end of one series of the algorithm and these sub-steps (Source, Convection, and Diffusion) are iteratively conducted in LG-MC.

3. Test Problem and Numerical Results

In this section, we present two results from the LG-MC code: coupled results of a convection-source problem and a result of a convection-conduction problem for the energy equation. The first

example was done only with LG, i.e., without MC scheme, to validate our numerical algorithm for the convective-part and the source-part in the system. The second example was done with LG-MC. To check the integrating algorithm of LG and MC, we solved the energy equation including convection and conduction terms.

1) coupled results of a convection-source problem

In this problem, Eqs. (1),(2), and (5) have been solved without the heat conduction term in Eq. (5). The calculation domain is set as a simple 1D SOL model geometry along the field line as shown in Fig. 1. Assuming uniformly distributed perpendicular particle/heat source from the core, the source terms have been set as;

$$S_n = S_0\theta(x_X - x), S_T = Q_0\theta(x_X - x), \tag{18}$$

where S_0 and Q_0 are the constant particle and heat source, respectively. The function $\theta(x)$ is the Heaviside step function and x_X represents the position of the X-point. The distance between the stagnation point and the divertor plate is $L_x = 100$ m and the X-point is located at $x = 70$ m. The grid resolution $\Delta x = 5.0$ m and the time step is $\Delta t = 2.29 \times 10^{-6}$ s. For the boundary condition, $V(\pm L_x) = \pm\sqrt{2T(\pm x_L)/m}$ is implemented. From the particle, momentum, and energy conservation laws, the numerical solution should satisfy following relations in steady state, if the problem is correctly solved.

$$nV = S_0 x(-x_X \le x \le x_X), nV = \pm S_0 x_X(x_X \le |x|). \tag{19}$$

$$mnV^2 + nT = mn(L_x)V(L_x)^2 + n(L_x)T(L_x) = \frac{3}{2}\sqrt{2mT(L_x)}S_0 x_X, T(L_x) = \frac{2Q_0}{7S_0}. \tag{20}$$

$$\frac{1}{2}mnV^3 + \frac{5}{2}nVT = Q_0 x(-x_X \le x \le x_X), \frac{1}{2}mnV^3 + \frac{5}{2}nVT = Q_0 x_X(x_X \le |x|). \tag{21}$$

The relation between the temperature and the velocity is;

$$T(V) = \frac{2Q_0}{5S_0} - \frac{1}{5}mV^2. \tag{22}$$

The results with $S_0 = 5.0 \times 10^{21}\mathrm{m}^{-3}\mathrm{s}^{-1}$ are shown in Fig. 1(a)-(e). Equations (19) to (22) were used for validation.

As shown in Fig. 1, the converged numerical results satisfy particle balance, and energy balance well. The total pressure in Fig. 1-(d) slightly deviates from the analytic value. Two small differences at $x \sim -70$m and at $x \sim 70$m are due to the step-function-form of the source profile. In the rest of the domain, the slight deviation probably caused by the numerical diffusion produced, because we use a constant profile in each cell. Although we have such small deviations, the results in Fig. 1 prove that LG surely works to obtain reasonable 1D results for the three coupled fluid equations at least for the convective and source terms.

2) a test result of a convection-conduction problem from the energy equation

To validate the integrated scheme of LG and MC, Eq.(5) was solved for the following conditions; $S_{T_i} = S_n = 0$, $n = Const.$, and $V = Const.$ The heat coefficient κ was given as $\kappa = \kappa_0 T^{\frac{5}{2}}$ and two Dirichlet boundary conditions were set as $T(0) = 10eV$, $T(L) = 1eV$. In the LG-MC scheme, as noted in Sec. 2, the conduction term is treated with the MC scheme while all other terms are treated with LG. It is also possible to include the conduction term into LG by changing the weight of temperature W_T for the Lagrange particles. Therefore, we solved the same test case as discussed before with only the LG scheme. In addition, a benchmark was also done for the same case with a finite-volume scheme (FV)[9]. The stationary results are shown in Fig. 2. For future applications in 2D and 3D the MC treatment of radial (anomalous) transport is anyhow needed, LG will be used along the field lines to avoid problems with the pressure gradient terms.

As seen from Fig. 2, the results from the three schemes(LG-MC, LG, and FV) agree well. The slight difference at the last calculation point near the right boundary originates from the different treatment of the boundary condition. The Dirichlet boundary condition, $T(L) = 1eV$,

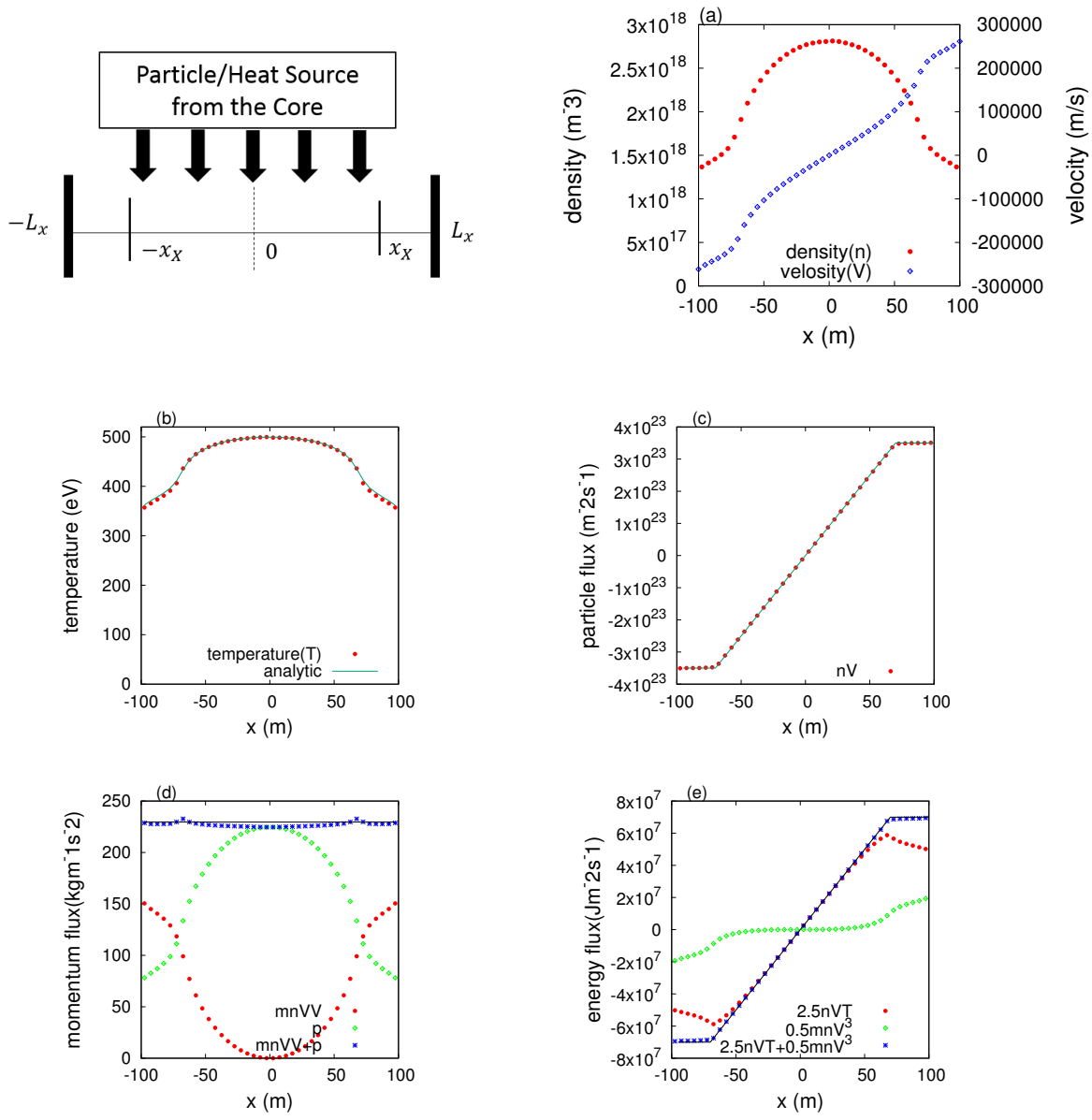

Fig 1: 1D SOL model and 1D results of the Lagrange scheme. (a)density and flow velocity. (b)Ion temperature. The line is the analytical solution of temperature calculated by Eq. (22) using the calculated velocity. (c)particle conservation. The lines are from Eq.(19). (d)momentum conservation. The line is the value calculated by Eq. (20). (e)energy conservation. The lines are from Eq. (21)

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is set exactly at the right wall in LG while it is set as a virtual "heat reservoir" at an additional cell placed outside of the wall in LG-MC. Although we should pay careful attention on this point in future benchmark problems, the result supports the validity of the LG-MC and the LG schemes.

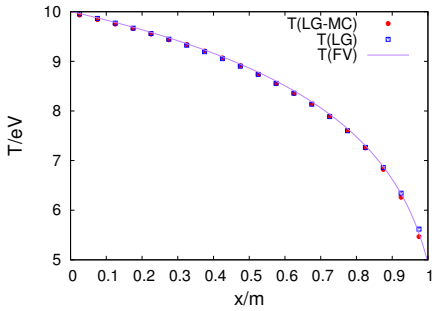

Fig 2: Result of the temperature profile obtained by LG-MC(red dots), LG(blue squares), and FV(solid line).

4. Summary and Future Plan

As a new numerical scheme for a plasma fluid code, the Lagrange-Monte-Carlo scheme (LG-MC) has been developed. To validate the algorithm of the scheme, we conducted two numerical tests; 1) a test for the Lagrange-scheme (LG) solving a coupled equations of particle, momentum and energy conservation with convection and source terms and 2) a test for LG-MC solving the energy equation with convection and conduction terms. The first case confirmed that particle, momentum, and energy conservation are reasonably satisfied. The second case confirmed the validity of the combined LG-MC scheme for solving the energy equation with convection and conduction. At present we extend the LG-MC scheme to solve a more realistic scenario. Afterwards, neutral sources/sinks will be added to reproduce a detached state and the code will be extended to 2D or 3D, which is relatively simple for particle methods.

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