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3D Monte Carlo modelling of edge plasmas in fusion experiments

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Abstract. A three-dimensional model for the numerical simulation of transport in the edge plasma of modern fusion devices is developed. The model is based on the Braginskii set of equations which are solved with the help of a Monte Carlo method by three-dimensional plasma transport code E3D. The multiple coordinate system approach and interpolated cell mapping technique used in E3D allow us to avoid artificial numerical cross-field transport due to a high anisotropy of Braginskii equations in the case of general magnetic configurations including ergodic regions. The complete self-consistent set of fluid equations (equations for the density, parallel momentum, ion and electron temperatures) has been successfully implemented in E3D. A stabilization method for iterating coupled momentum and density equations is discussed.

1. Introduction

The present generation of fusion experiments—both for tokamaks and stellarators—requires the development of advanced theoretical models. The aim of this work is to develop a general three-dimensional (3D) model for the numerical simulation of transport of the edge plasma in modern fusion devices. An important point here is the accurate description of regions with complex (eventually ergodic) topology of the magnetic field lines. Such structures are expected both in tokamaks (e.g. in TEXTOR during ergodic divertor operation [1] or in DIII-D with additional coils [2]) and in stellarators. The transport model is based on the Braginskii hydrodynamic set of equations [3]. In our earlier work [4, 5], heat conductivity equations only have been solved for a 3D geometry. Here, these equations have been complemented by continuity and momentum conservation equations. The peculiarities of the Monte Carlo method for the solution of these last two equations are described below.

2. Solution of Braginskii equations by a Monte Carlo method

One of the main problems in the numerical solution of Braginskii equations is the anisotropy of transport along and across the magnetic field: the corresponding

transport coefficients differ by a factor of 10^6–10^8, which makes the system numerically stiff. In our case of general magnetic geometry we introduce a coordinate system linked to the magnetic field lines in order to separate parallel and perpendicular transport and, therefore, to avoid possible numerical diffusion. Here 'numerical diffusion' means the numerically induced contribution of (very large) parallel transport to transport in the perpendicular direction. It is easy to see that if we choose a coordinate system (x^1, x^2, x^3) with x^3 aligned to the field line ($\mathbf{h}\cdot\nabla x^i = 0$, $i = 1, 2$, $\mathbf{h} \equiv \mathbf{B}/B$) there is a contribution of the parallel transport in the element D^{33} of the diffusion tensor only. On the other hand, the contribution of the perpendicular transport to the parallel transport is negligible.

This coordinate system is non-periodic, i.e. in the general case it is impossible to construct a mesh which would match itself exactly after a toroidal period. Therefore, some kind of interpolation is necessary, which, again, can lead to the contribution of parallel transport in the perpendicular direction.

It should be noted that the usage of several coordinate systems called local magnetic coordinate systems (LMCSs) is also possible. The number of LMCSs depends on the problem solved, e.g., for the case of the ergodic magnetic field layer, the scope of a single system should be at least well below the Kolmogorov length.

There are two direct ways to avoid the problem of matching mentioned above: first, to construct a special irregular mesh which matches itself approximately; second, to solve the problem with the help of a Monte Carlo method using an interpolated cell mapping procedure to join the non-matching ends of the coordinate system (see [4] and references therein for details). Here, we treat the second possibility only.

All Braginskii equations have the following convection-conduction form,

$$\frac{\partial f}{\partial t} - \frac{1}{\sqrt{g}}\frac{\partial}{\partial x^i}\sqrt{g}\left(D^{ij}\frac{\partial f}{\partial x^j} - V^i f\right) = S - \nu f. \tag{2.1}$$

Therefore, they can be solved with the help of a random walk procedure. Here, V^i is convection velocity, g is the metric determinant and D^{ij} is the diffusion tensor appropriate for a generalized 'fluid quantity' f, $D^{ij} = [D_\perp g^{ij} + (D_\parallel - D_\perp)h^i h^j]$, where $g^{ij} = (\nabla x^i)\cdot(\nabla x^j)$. An explicit form of (2.1) in local magnetic coordinates is given in [4].

Electron and ion energy equations can be solved by this method efficiently due to the optimized coordinates introduced in [5], which remove the limitation of the parallel step by the parallel scale of the magnetic field. The solution of the 'dynamic' part of the system (continuity and momentum equations) is not so straightforward.

First of all, in contrast to the temperature, parallel momentum can be both, positive and negative. Therefore, it has to be modelled by random walks of two species of particles, positive and negative momentum carriers. Representing pressure gradient, which is, generally, polluted by noise in Monte Carlo calculations, by local sources of positive and negative momentum carriers, unlimited growth of the total amount of particles must be prevented by adding conditional sinks into equations for momentum carriers. Denoting densities of positive and negative carriers with n^+ and n^-, respectively, the same sink term, $\nu_{\text{sink}} n^+ n^- / (n^+ + n^- + n_{\min})$, is added into equations for both carriers. Here ν_{sink} is a sink rate, $n_{\min}$ is some limiting density and $n^\pm$ are carrier densities from the previous iteration. These sinks cancel each other in the momentum equation and, therefore, affect only momentum carrier densities but not the momentum density itself.

Second, solution of coupled momentum and density equations by means of simple successive iterations requires a method which enforces stability. Let us analyze a homogeneous linearized one-dimensional (1D) problem at the infinite interval using the von Neumann method. The unperturbed parallel velocity is assumed to be zero (therefore, the most severe problem which appears near stagnation points is considered). Thus, perturbation of the momentum density is $p_\parallel \approx m_\mathrm{i} n_0 V$, where V is the velocity perturbation. The unperturbed density, n_0, and temperatures are assumed constant, $T_\mathrm{e} + T_\mathrm{i} = m_\mathrm{i} C_\mathrm{s}^2 = \text{constant}$, were C_s is a sound speed. The linearized 1D set of equations is

$$\frac{\partial n}{\partial t} = -n_0 \frac{\partial}{\partial x} V,$$
$$\frac{\partial V}{\partial t} - D_V \frac{\partial^2}{\partial x^2} V = -\frac{C_\mathrm{s}^2}{n_0} \frac{\partial n}{\partial x}, \tag{2.2}$$

where n is density perturbation and D_V is parallel velocity diffusion coefficient due to the viscosity. Using Fourier analysis of the perturbed quantities over the coordinate, $n, V \propto \exp(ikx)$, equation set (2.2) is transformed to

$$\frac{\partial n}{\partial t} = -ikn_0 V, \tag{2.3}$$
$$\frac{\partial V}{\partial t} + k^2 D_V V = -ik \frac{C_\mathrm{s}^2}{n_0} n. \tag{2.4}$$

This set is solved by subsequent integrations of each equation at each iteration ('time step' Δt). Let n_m and V_m be density and velocity perturbations after m time steps. The recurrence relation in matrix form is

$$\begin{pmatrix} n_{m+1} \\ V_{m+1} \end{pmatrix} = \begin{pmatrix} 1 & -ikn_0 \Delta t \\ -ik \frac{C_\mathrm{s}^2}{n_0} \tau_V & \theta_V - k^2 C_\mathrm{s}^2 \Delta t \tau_V \end{pmatrix} \begin{pmatrix} n_m \\ V_m \end{pmatrix} \equiv \mathbf{A} \cdot \begin{pmatrix} n_m \\ V_m \end{pmatrix}, \tag{2.5}$$

where $\tau_V = (1 - \theta_V)/(k^2 D_V)$, and $\theta_V = \exp(-k^2 D_V \Delta t)$. Stability of iterations is determined by eigenvalues of matrix $\mathbf{A}$ which are defined by the characteristic equation $\det(\mathbf{A} - \lambda \mathbf{I}) = 0$ where $\mathbf{I}$ is a unit matrix,

$$\lambda^2 - \mathrm{Sp}(\mathbf{A})\lambda + \det(\mathbf{A}) = \lambda^2 - (1 + \theta_V - b)\lambda + \theta_V = 0, \tag{2.6}$$

$$b = k^2 C_\mathrm{s}^2 \Delta t \tau_V. \tag{2.7}$$

Iterations are stable, if $|\lambda|^2 < 1$. In our case this condition means

$$C_\mathrm{s}^2 \Delta t (1 - \theta_V)/D_V > 2(1 + \theta_V). \tag{2.8}$$

Estimating $D_V \sim C_\mathrm{s}^2 \tau_\mathrm{i}$, where τ_i is ion–ion collision time, and taking into account that $0 < \theta_V < 1$, instability is obtained if $\Delta t \geqslant \tau_\mathrm{i}$. This is a very restrictive condition which requires an extremely large number of iteration steps.

In order to overcome this difficulty in a steady state problem, under-relaxation factors, $0 < r_n < 1$ and $0 < r_V < 1$, are introduced for the density and velocity, respectively. Namely, instead of using (2.5), new values of density and velocity are taken in the form $X_\mathrm{new} = rX_\mathrm{old} + (1 - r)X'$, where X' is the new value of X without the under-relaxation. Introducing this modification into the recurrence relation (2.5), stability analysis described by (2.6)–(2.8) remains the same up to a replacement of θ_V and b with $\theta'_V = r_V + (1 - r_V)\theta_V$ and $b' = (1 - r_n)(1 - r_V)b$, respectively. Therefore, iterations are stable as long as $(1 - r_n)(1 - r_V)\Delta t < \tau_\mathrm{i}$, which

practically removes the limitation on the iteration time step Δt because the factor $(1-r_n)(1-r_V)$ can be made small. On the other hand, this factor should not be too small because this would, again, increase the number of iterations: contribution of the first iteration to the final result decays as $\exp(-(1-r)M)$ where M is the total number of iterations, and iterations converge when this contribution is negligibly small. Therefore, optimum values of under-relaxation factors are such that they allow Δt of the order of the profile relaxation time.

Under-relaxation factors also allow us to reduce the variance. Denoting the variance at a single iteration step with σ^2, presenting the under-relaxation factor as $r = 1-1/N$ where $N \gg 1$ and assuming that statistical errors at different iterations are statistically independent, the variance for an infinite number of iterations is obtained as

$$\sigma_\infty^2 = \frac{\sigma^2}{2N}\frac{1}{1-1/(2N)} \to \frac{\sigma^2}{2N}.$$

Practically, it is sufficient to make such a number of iteration steps, M, that the variance from the first iteration decays to the level of σ_∞, i.e. $\sigma^2 \exp(-(1-r)M) = \sigma_\infty^2$. This relation gives the optimum number of iterations for a given under-relaxation factor,

$$M = \frac{N}{2}\log(2N) = \frac{1}{2(1-r)}\log\left(\frac{2}{1-r}\right).$$

Practical realization of the under-relaxation in the Monte Carlo algorithm assumes that the distribution of quantity X given by the density of test particles at the end of an iteration step is replaced with the under-relaxated distribution (see above). Such a procedure means that the re-discretization of quantity X has to be performed after each iteration. In a 3D case, this re-discretization procedure introduces the numerical cross-field transport due to the averaging within the parameter mesh cells. The effective numerical diffusion coefficient is $h^2/\Delta t$ where h is the perpendicular size of the mesh cells. If the iteration time step Δt is large enough (e.g. comparable with the optimum step which is of the order of the profile relaxation time), this numerical diffusion is negligibly small.

3. Conclusions

Stabilization method for iterating coupled momentum and density equations has been implemented in the 3D fluid Monte Carlo code E3D. The results of the first run for the unperturbed DIII-D magnetic configuration using $r_n = r_V = 0.99$ are in qualitative agreement with 2D calculations. The convergence time for this run was around 24 hours on 64 processors at the PC cluster at MPI Greifswald which is a practically acceptable time. Thus, the complete self-consistent set of fluid equations (equations for the density, parallel momentum, ion and electron temperatures) has been successfully implemented in E3D.

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