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# Transport in complex magnetic geometries: 3D modelling of ergodic edge plasmas in fusion experiments

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#### Abstract

Both stellarators and tokamaks can have quite complex magnetic topologies in the plasma edge. Special complexity is introduced by ergodic effects producing stochastic domains. Conventional numerical methods from fluid dynamics are not applicable in this case. In the present paper, we discuss two alternative possibilities. Our multiple coordinate system approach (MCSA) [Phys. Plasmas 8 (2001) 916] originally developed for the TEXTOR DED allows modelling of plasma transport in general magnetic field structures. The main idea of the concept is: magnetic field lines can exhibit truly stochastic behavior only for large distances (compared to the Kolmogorov length), while for smaller distances, the field remains regular. Thus, one can divide the computational domain into a finite set of sub-domains, introduce local magnetic coordinate systems in each and use an 'interpolated cell mapping' technique to switch between the neighboring coordinate systems. A 3D plasma fluid code (E3D, based upon MCSA) is applied to realistic geometries. We also introduce here some new details of the algorithm (stellarator option). The results obtained both for intrinsic (stellarator) and external (tokamak with ergodic divertor) perturbations of the magnetic field are discussed. Another approach, also using local coordinate systems, but based on more conventional finite difference methods, is also under development. Here, we present the outline of the algorithm and discuss its potential as compared to the Lagrangian Monte-Carlo approach.

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#### 1. Introduction

The new generation of fusion devices – both stellarators and tokamaks – are being built with very complicated topology of the field lines [2,3], including intact magnetic surfaces, island chains, ergodic and laminar zones. Ergodic effects can be an intrinsic property (e.g.

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in W7-X, due to finite  $\beta$  effects) or can be caused by externally applied 'ergodic divertors' (e.g. TEXTOR DED). The key point for a quantitative assessment of plasma edge and surface effects under such conditions is a formally correct computational description also of the regions with fully or partially developed ergodic magnetic field structure. This leads to difficulties in edge plasma modelling compared to the 'classical' tokamak divertor: the problem becomes essentially 3D (i.e., one can only poorly represent the magnetic geometry by a toroidally averaged grid [4]). In addition, partly developed ergodicity prevents the usage of some 'global'

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magnetic coordinate system aligned to magnetic surfaces since these surfaces do not exist anymore. It should be noted that such a non-regular behaviour of the magnetic field lines in the stellarator periphery is rather a rule: even in the same device, with increased plasma pressure, ergodic layers may appear at the location of former regular islands [11]. The existing 3D plasma edge codes are usually restricted to the case of weak perturbation (spectral methods [10]) or regular magnetic geometry (intact islands [7,9]), see Ref. [1] for a more detailed discussion.

In our previous work [1] we have presented our 3D plasma fluid code (E3D) addressing this matter. E3D is a 3D scrape-off-layer plasma transport code under development to solve a system of plasma fluid equations in this general magnetic geometry. It is a fluid Monte-Carlo code based upon our multiple coordinate system approach (MCSA, see Ref. [1]). The main idea of the concept is: magnetic field lines can exhibit truly stochastic behavior only at large distances (compared to the Kolmogorov length, i.e. the characteristic length of the exponential divergency of two initially neighboring starting points), while for smaller distances, the field lines remain regular. Thus, one can divide the computational domain into a finite set of sub-domains, introduce local magnetic coordinate systems in each and use an 'interpolated cell mapping' technique to switch between the neighboring coordinate systems. The method has been successfully benchmarked in a non-trivial case (single island geometry) against the 3D finite-volume code BoRiS [12]. E3D was originally developed for tokamak ergodic divertors (TEXTOR-94) and is currently being extended toward stellarator applications (W7-X). Here, we present some geometrical improvements of the algorithm. We restrict ourselves to the conduction part of the electron energy equation, assuming constant plasma density.

An alternative numerical realization of the idea of MCSA (based upon a finite-difference scheme) is also being investigated. The major problem to be overcome is the problem of properly closing the discretization of the grid created by field line tracing.

In Section 2 we summarize the main ideas of MCSA and introduce the transport model equation used further. In Section 3 we formulate our modifications of the geometry (stellarator option) and discuss the alternative numerical approach mentioned above. In Section 4, we present and discuss the first results for W7-X.

# 2. Transport model

Following Ref. [1], we restrict ourselves to the heat balance equation for electrons, neglecting convection for simplicity:

$$\frac{\partial}{\partial t} \frac{3}{2} nT - \nabla \cdot \left[ \kappa_{\perp} \nabla T + (\kappa_{\parallel} - \kappa_{\perp}) \mathbf{h} \mathbf{h} \cdot \nabla T \right] = 0. \tag{1}$$

Here T stands for the electron temperature, n is the plasma density (further assumed to be constant),  $\mathbf{h} = \mathbf{B}/B$  is a unit vector along the magnetic field,  $\kappa_{\perp}$  and  $\kappa_{\parallel}$  are the anomalous (usually constant) perpendicular and classical parallel thermal conductivity coefficients, respectively.

In general curvilinear coordinates  $x^i$ , Eq. (1) can be written in the following form:

$$\frac{\partial T}{\partial t} = \frac{1}{\sqrt{g}} \frac{\partial}{\partial x^i} \sqrt{g} \left( D^{ij} \frac{\partial T}{\partial x^j} \right). \tag{2}$$

Here g is the metric determinant and  $D^{ij}$  is the diffusion tensor appropriate for T,

$$D^{ij} = \frac{2}{3} [\chi_{\perp} g^{ij} + (\chi_{\parallel} - \chi_{\perp}) h^i h^j], \tag{3}$$

where  $g^{ij} = (\nabla x^i) \cdot (\nabla x^j)$  and  $h^i = \mathbf{h} \cdot \nabla x^i$  are contravariant components of the metric tensor and of the unit vector along the magnetic field, respectively, while  $\chi_{\perp} \equiv \kappa_{\perp}/n$  and  $\chi_{\parallel} \equiv \kappa_{\parallel}/n$ .

In Ref. [1], we proposed a general class of possible coordinate systems which permits strict separation of perpendicular and parallel fluxes (being different by several orders of magnitude for typical plasma parameters). This is the type of coordinate systems that are used in fusion plasma analysis to construct magnetic stream functions (Clebsch coordinates). For such a coordinate system, the minimum requirement is that the first two variables  $x^i$  must satisfy the magnetic differential equation,

$$\mathbf{h} \cdot \nabla x^i = 0, \quad i = 1, 2, \tag{4}$$

while the third variable,  $x^3$ , is an angle-like variable which is increasing along the magnetic field lines,

$$\mathbf{h} \cdot \nabla x^3 > 0. \tag{5}$$

Hence, we require that the covariant base vector  $\mathbf{e}_3$  point along the magnetic field line, i.e. the parallel flux has only one non-vanishing component.

Generally, we are forced to restrict the scope of a single coordinate system by some proper length (the theoretical limit here is the Kolmogorov length), hence the use of local magnetic coordinates.

We couple the neighboring coordinate systems with the help of an 'interpolated cell mapping' technique (a precomputed transformation of lines  $x^1 = \text{constant}$  and  $x^2 = \text{constant}$ , interpolated by means of bicubic splines). By increasing the mesh resolution within practically available computer memory limits, one can reduce the errors introduced by this kind of ICM to the level of the direct field line tracing error.

To specify a local magnetic coordinate system, one needs initial conditions for Eq. (4). In general, these can be any two one-parametric families of curves on some surface which is never tangential to the magnetic field (reference cut). In [1] we used a 2D Cartesian mesh for this purpose. A good choice of the coordinates  $x^1, x^2$  is a non-trivial task for stellarator applications. We will treat this subject in Section 3.

## 3. Stellarator geometry

We introduce two essential geometrical improvements in this section: first, we optimize the choice of basis curve families being the initial conditions for Eq. (4); second, we reduce the number of our local coordinate systems to the minimum possible (1 in this particular case) to speed up our calculations.

In the previous version of the code, the number of coordinate systems was chosen large enough, such that the variation of metric coefficients along the magnetic field lines was small within the domain of a particular coordinate system. However, this limitation may be stronger than the requirement of relatively simple topology of the magnetic field near the wall. The excessive number of coordinate systems causes the overuse of memory and slows down the algorithm, because many changes of coordinate systems may be necessary for

advancing a test particle by one time step. In the present realization of the code, the number of coordinate systems is not linked to the parallel scale of the metric tensor anymore.

In the case of a stellarator, simple Cartesian (or polar) meshes are an unnatural basis for the families of coordinate planes because of the more complicated shape of the magnetic surfaces (wherever they exist). Indeed, one should be able to reproduce at least the last closed magnetic surface and the wall very precisely to pose reasonable boundary conditions. The idea here is: we do not intend to (nor can) reproduce magnetic surfaces exactly in case of ergodicity, but we try to cover the configuration with our mesh as efficiently as possible. Let us choose the section  $\varphi = \varphi_{\rm m} \equiv \pi/5$  ('triangular' section) as a reference cut, and require that our inner boundary (to the core plasma) exactly coincide with some closed magnetic surface at the edge. As the outer boundary we use here an outer closed magnetic surface (existing in this particular case, see Fig. 1(a)), and introduce the 'radial' variable  $\rho$  as a coefficient of linear interpolation in between. (Probably, the wall itself could be the better choice as the outer boundary of computational domain, and we plane this improvement for the future.) The natural choice of the second one is the VMEC angle-like poloidal variable  $\vartheta_V$  (see Ref. [8] for details). Further we will refer to this mesh as 'quasimagnetic' (QM). It is defined through cylindrical coor-

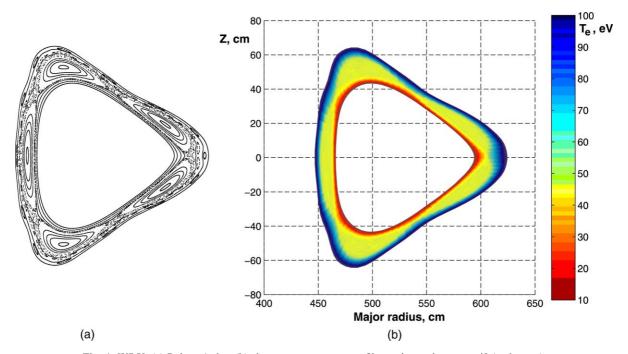


Fig. 1. W7-X: (a) Poincaré plot; (b) electron temperature profile on the section  $\varphi = \pi/5$  (real space).

dinates as follows. We have both closed magnetic surfaces in form of a Fourier expansion over VMEC angles:

$$R_{\rm in} \equiv R_{\rm in}(\vartheta_{\rm V}, \varphi), \quad R_{\rm out} \equiv R_{\rm out}(\vartheta_{\rm V}, \varphi),$$
  

$$z_{\rm in} \equiv z_{\rm in}(\vartheta_{\rm V}, \varphi), \quad z_{\rm out} \equiv z_{\rm out}(\vartheta_{\rm V}, \varphi).$$
(6)

The VMEC angle  $\varphi$  is the same as the toroidal angle of cylindrical coordinates. We have explicit transformation formulas from the OM to Cartesian mesh:

$$R = Q^{1}(\rho, \vartheta_{V}, \varphi) = \rho R_{\text{out}}(\vartheta_{V}, \varphi) + (1 - \rho)R_{\text{in}}(\vartheta_{V}, \varphi),$$

$$z = Q^{2}(\rho, \vartheta_{V}, \varphi) = \rho z_{\text{out}}(\vartheta_{V}, \varphi) + (1 - \rho)z_{\text{in}}(\vartheta_{V}, \varphi).$$
(7)

Here  $0 \le \rho \le 1$ . The inverse transformation is given by functions  $\mathbf{P} \equiv \mathbf{Q}^{(-1)}$ ,

$$\rho = P^1(R, z, \varphi) \quad \text{and} \quad \vartheta_V = P^2(R, z, \varphi).$$
(8)

These functions are obtained by the numerical inversion of the set of non-linear algebraic equations (7) and are needed only at the reference cut  $\varphi = \varphi_m$ .

Using the usual tensor algebra rule,

$$g_{\text{new}}^{ij} = g_{\text{old}}^{kl} \frac{\partial x_{\text{new}}^i}{\partial x_{\text{old}}^k} \frac{\partial x_{\text{new}}^j}{\partial x_{\text{old}}^l}, \tag{9}$$

the metric tensor of cylindrical coordinates is transformed to local magnetic coordinates through subsequent changes of the following coordinate systems:

(1) cylindrical coordinates  $\mathbf{y} \equiv (y^1, y^2, y^3) = (R, z, \varphi)$ ;

- (2) local magnetic coordinate system with Cartesian mesh as the base curves  $\mathbf{v} = (v^1, v^2, v^3)$ ;
- (3) local magnetic coordinate system with QM as the base curves  $\mathbf{x} \equiv (x^1, x^2, x^3)$ .

The first and second coordinate systems are linked by the field line (orbit) integration using a method similar to Refs. [5,6]. All three systems have (almost) the same third coordinate,  $y^3 \equiv \varphi$  and  $x^3 \equiv v^3 \equiv \varphi - \varphi_{\rm m}$ . It means, the local magnetic coordinate systems (2) and (3) are simply linked by Eqs. (7), (8) (replacing (R,z) with  $(v^1,v^2)$  and  $(\rho,\vartheta_V)$  with  $(x^1,x^2)$ ).

The finite difference code makes use of an optimized grid which has to be constructed to minimize numerical diffusion: the basic idea is to use only those field lines which get so close back to their starting points that the numerical diffusion is sufficiently small, i.e. satisfying  $\Delta \ll L_{\parallel} \sqrt{\chi_{\perp}/\chi_{\parallel}}$ , where  $\Delta$  is the excursion between the start and end points on the cut and  $L_{\parallel} \approx 2\pi RN$  is the distance between the same points measured along the field line (N is the number of toroidal turns). For the parameters we use to construct the W7-X grid ( $\Delta = 1$ mm, N = 50/100 by plasma radius about 0.5 m), the induced numerical diffusion is of the order  $10^{-4}$  m<sup>2</sup>/s, i.e. negligible compared to the physical  $\chi_{\perp}$ . The physics argument for the procedure discussed above is that if this excursion between the two points gets below one ion gyroradius (which is of the order of 1 mm) one should not expect physics differences. It then solves the transport equations using local magnetic coordinates. The transport contributions on the toroidal cuts are discretized by Delauney triangulation. For this, the flux

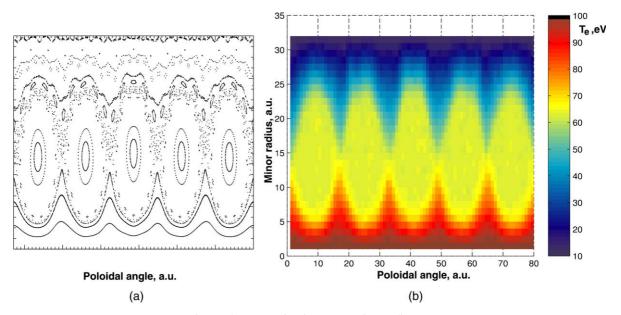


Fig. 2. The same as in Fig. 1, magnetic coordinates.

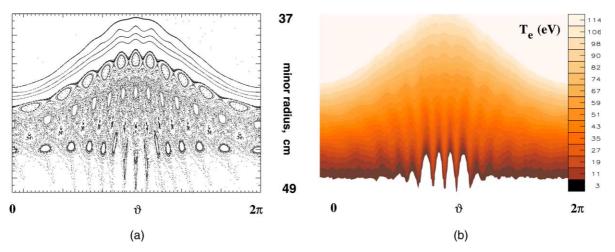


Fig. 3. The same for TEXTOR, polar coordinates.

balances based on Voronoi cells are solved and a finite-difference discretization is obtained by dividing through the control volumes (see Ref. [13] for details of the numerical method). The remaining terms, where variations along the field lines are treated, are discretized with central differences. First results for 1D, 2D and simplified 3D cases were obtained and a grid for W7-X was constructed. The potential of this model lies in the fact that, instead of the computational expensive Monte-Carlo estimate, optimized numerics (e.g. solvers, preconditioners) can be used. In comparison with finite volume methods, one does not have the problem of constructing 3D computational cells (which in ergodic systems get more and more distorted and have to cover the full domain to guarantee flux conservation).

## 4. Results and discussion

The improved MC method described above is applied to W7-X (Fig. 1 and 2), demonstrating the general applicability of our method. We solve the Eq. (2) in a low- $\beta$  case with prescribed electron temperatures at both boundaries (100 and 10 eV, respectively). Qualitatively, the results are similar to our previous calculations for the ergodic divertor of TEXTOR-94 (Fig. 3): the structure of the magnetic field (see Poincaré maps (a)) modulates strongly the temperature field (b).

This corresponds to the effect of a component of fast parallel transport in the radial direction. It should be noted that, unlike in our previous publication [1], the magnetic field of TEXTOR-94 used in the results presented in Fig. 3, is based on calculations taking into account the real coil system instead of analytical model, but with our 'old' ideology of the choice of coordinates [1].

The small stochasticity in the low- $\beta$  case of W7-X leads to some 'heat leakage' (enhanced energy transport towards the wall) in the vicinity of the X-points. One can expect an increase of this effect with higher plasma pressures. Further work for W7-X is necessary to analyze cases with stronger ergodicity (higher  $\beta$ ) and to include the complete geometry (vessel walls, limiters, target plates, ...). An extension of this work to the full set of transport equations is then the final step.

### 5. Conclusions

E3D is approaching a level of maturity for general applicability: the geometry of the code is generalized to various applications (W7-X, TEXTOR, etc.) Calculations for heat conduction in real W7-X and TEXTOR geometries demonstrate that the structure of the magnetic field strongly modulates the temperature field. The small stochasticity in the low- $\beta$  case of W7-X leads to some 'heat leakage' in the vicinity of X-points.

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