

Extensions of the 3-Dimensional Plasma Transport Code E3D

A. Runov^{*1}, S. Kasilov², R. Schneider¹, and D. Reiter³

¹ Max-Planck Institut für Plasmaphysik, EURATOM Association, D-17491 Greifswald, Germany

² Institut of Plasma Physics, National Science Center “Kharkov Institute of Physics and Technology”, 61108, Kharkov, Ukraine

³ Institut für Plasmaphysik, Forschungszentrum Jülich GmbH, EURATOM Association, Trilateral Euregio Cluster, D-52425 Jülich, Germany

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One important aspect of modern fusion research is plasma edge physics. Fluid transport codes extending beyond the standard 2-D code packages like B2-Eirene or UEDGE are under development. A 3-dimensional plasma fluid code, E3D, based upon the Multiple Coordinate System Approach and a Monte Carlo integration procedure has been developed for general magnetic configurations including ergodic regions. These local magnetic coordinates lead to a full metric tensor which accurately accounts for all transport terms in the equations. Here, we discuss new computational aspects of the realization of the algorithm.

The main limitation to the Monte Carlo code efficiency comes from the restriction on the parallel jump of advancing test particles which must be small compared to the gradient length of the diffusion coefficient. In our problems, the parallel diffusion coefficient depends on both plasma and magnetic field parameters. Usually, the second dependence is much more critical. In order to allow long parallel jumps, this dependence can be eliminated in two steps: first, the longitudinal coordinate x^3 of local magnetic coordinates is modified in such a way that in the new coordinate system the metric determinant and contra-variant components of the magnetic field scale along the magnetic field with powers of the magnetic field module (like in Boozer flux coordinates). Second, specific weights of the test particles are introduced. As a result of increased parallel jump length, the efficiency of the code is about two orders of magnitude better.

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1 Introduction

In Ref. [1], a Monte Carlo approach has been proposed for the modelling of particle and energy transport in three-dimensional (3D) magnetic fields of general topology which may include regions with embedded magnetic surfaces as well as regions with islands and ergodic magnetic field lines. This approach is based on the fact that fluid transport equations are of parabolic type pertinent to the diffusion problem. Therefore, we can use the analogy between the transport phenomena in plasmas and the random walk of Brownian particles which satisfies the Fokker-Planck equation. For this purpose, fluid parameters such as particle density, energy density, etc. can be represented as a weighted density of test particles, and we specify the coefficients of the Fokker-Planck equation in accordance with the transport coefficients of the original equation. Such a Monte Carlo approach to diffusion-like equations is a conventional computational method. At the same time, the problem of plasma transport has a specific feature connected with a strong anisotropy of transport coefficients: parallel and perpendicular heat conductivity coefficients differ by several orders of magnitude. It is an essential difficulty to any numerical method applied to transport equations in real space coordinates. Therefore, in two-dimensional (2D) [2] and 3D [3] modeling of plasma transport with finite-difference methods a system of magnetic flux coordinates is used where one of the coordinates (flux label) remains unchanged along the magnetic field lines. Such a coordinate system allows us to separate the fast process of plasma transport along the magnetic field from the slow cross-field transport into different coordinates and therefore to avoid numerically induced cross-field transport. However,

* Corresponding author: e-mail: runov@ipp.mpg.de, Phone: +49 3834 882432, Fax: +49 3834 882409

in a general case of the magnetic field topology, it is impossible to introduce a single valued flux label. For this general case, a Multiple Coordinate System Approach (MCSA) has been proposed in Ref. [1] where sets of magnetic coordinates (x^1, x^2, x^3) such that

$$\mathbf{h} \cdot \nabla x^1 = \mathbf{h} \cdot \nabla x^2 = 0 \quad (1)$$

(here \mathbf{h} is a unit vector along the magnetic field) are introduced independently in different subdomains. These coordinate sets do not have simple periodicity properties, like flux coordinates. However, this absence of simple periodicity does not affect the accuracy of Monte Carlo procedures where the coordinates of test particles can be accurately transformed from one local magnetic coordinate set (LMCS) to another if the particle travels to the next (previous) spatial subdomain. For this purpose the Interpolated Cell Mapping (ICM) technique is used where high accuracy of coordinate transformation is achieved by means of bi-cubic splines. Based upon MCSA, the Monte Carlo code E3D has been developed and applied to the problem of heat conductivity in the Dynamic Ergodic Divertor (DED) of the tokamak TEXTOR [1]. This code has been successfully benchmarked with a 3D finite-volume code BoRiS [4] in the case of a single island geometry. MCSA is also an essential part of a different Monte Carlo procedure, Stochastic Mapping Technique (SMT), which is used to solve the drift kinetic equation in the long-mean-free-path regime in toroidal fusion devices [5].

In [6] we proposed some optimizations of the coordinate system for the stellarator case. Here, we present further optimisation of the numerical procedure which improves the efficiency of the algorithm fundamentally: The restriction on the time step in Monte Carlo is obvious - a single particle step must be small compared to the gradient length of the diffusion coefficient. Here, the parallel diffusion coefficient depends on both plasma and magnetic field parameters. The plasma parameter dependence comes through the non-linear parallel heat conduction, whereas the magnetic field dependence comes through h^3 and the metric determinant. To allow for long parallel steps, magnetic field dependencies must be eliminated. We achieve this in two steps: first, the longitudinal coordinate x^3 of the local magnetic coordinates is modified in such a way that in the new coordinate system the metric determinant and contra-variant components of the magnetic field scale along the magnetic field with powers of the magnetic field module (like in Boozer flux coordinates) (Section 2). Second, we introduce specific weights of the test particles (Section 3).

2 New parallel coordinate

Let us recall the main ideas of Refs. [1], [6]. Formally, in fluid dynamics we deal with this convection-conduction differential equation for some generalised "fluid quantity" u in the form of a conservation law:

$$\frac{\partial u}{\partial t} = \nabla \cdot (\mathbf{D} \cdot \nabla u - \mathbf{V}u) - \nu u + S_u = -\nabla \cdot \mathbf{F} - \nu u + S_u, \quad (2)$$

$$\mathbf{D} = D_{\perp} \mathbf{I} + (D_{\parallel} - D_{\perp}) \mathbf{h} \mathbf{h}, \quad \mathbf{F} = -\mathbf{D} \cdot \nabla u + \mathbf{V}u, \quad (3)$$

where \mathbf{D} and \mathbf{I} are diffusion and unit tensors respectively, \mathbf{h} is the unit vector along the magnetic field, and \mathbf{F} is a flux density, D_{\perp} and D_{\parallel} are the anomalous (usually constant) perpendicular and classical parallel generalised diffusion coefficients.

In general curvilinear coordinates x^i equation (2) can be written in the following form:

$$\frac{\partial u}{\partial t} - \frac{1}{\sqrt{g}} \frac{\partial}{\partial x^i} \sqrt{g} \left(D^{ij} \frac{\partial u}{\partial x^j} - V^i u \right) = S - \nu u. \quad (4)$$

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

$$D^{ij} = [D_{\perp} g^{ij} + (D_{\parallel} - D_{\perp}) h^i h^j], \quad (5)$$

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. If we choose a coordinate system like (1) (in which the magnetic field has only one nonzero component), we guarantee the separation of the parallel and perpendicular fluxes (i.e.

if $h^1 = h^2 = 0$, we have a contribution from D_{\parallel} in D^{33} only). Here, the parallel diffusion coefficient depends on both plasma and magnetic field parameters:

$$D_{\perp}^{ij} = D_{\perp} \left[g^{ij} - (h^3)^2 \delta_3^i \delta_3^j \right], \quad D_{\parallel}^{33} = D_{\parallel} (h^3)^2, \quad (6)$$

$$V_{\perp c}^i = \mathbf{V}_{\perp} \cdot \nabla x^i + \frac{1}{\sqrt{g}} \frac{\partial}{\partial x^j} \sqrt{g} D_{\perp}^{ij}, \quad V_{\parallel c}^3 = V_{\parallel} h^3 + \frac{1}{\sqrt{g}} \frac{\partial}{\partial x^3} \sqrt{g} D_{\parallel}^{33}. \quad (7)$$

The problem arises near the inner boundary of the domain: here there is a high constant temperature resulting in very large parallel heat conduction, while the characteristic length of the magnetic field is one period or even the distance between the coils, and this distance restricts the parallel jump of a particle. This means, that reproducing this constant temperature numerically will be very CPU intensive.

To eliminate the effects of magnetic field dependence in the last term in the second part of Eq.(7), let us introduce the new parallel coordinate as follows,

$$x_{(m)}^3 = S_{(m)} \int_{\varphi_{min}^{(m)}}^{\varphi} d\varphi' \frac{(B)^2}{B^{\varphi}} + \varphi_{min}^{(m)}. \quad (8)$$

Here, the integration is along the magnetic field line, $x^1 = const$, $x^2 = const$ (thus, $\varphi = x^3$), B is the magnetic field module, $B^{\varphi} = B^3$ - contra-variant toroidal (= parallel) component of the magnetic field, $\varphi_{min}^{(m)}$ is the lower boundary of the domain of m -th Local Magnetic Coordinate System (LMCS). The scaling factor which keeps the new coordinate in the fixed range $[\varphi_{min}^{(m)}, \varphi_{max}^{(m)}]$ is

$$S_{(m)} = \left(\varphi_{max}^{(m)} - \varphi_{min}^{(m)} \right) \left(\int_{\varphi_{min}^{(m)}}^{\varphi_{max}^{(m)}} d\varphi' \frac{(B)^2}{B^{\varphi}} \right)^{-1}, \quad (9)$$

where $\varphi_{max}^{(m)}$ is the upper boundary of the domain of m -th LMCS. One should now recall the property of the Jacobian of LMCS to scale inversely with B^3 (due to Gauss' law) in order to check that

$$\frac{\partial}{\partial x_{(m)}^3} \sqrt{g} (h^3)^2 = C(x^1, x^2) \frac{\partial}{\partial x_{(m)}^3} \frac{1}{B^3} (h^3)^2 = C(x^1, x^2) \frac{\partial}{\partial x_{(m)}^3} \frac{B^{\varphi}}{(B)^2} \frac{\partial x_{(m)}^3}{\partial \varphi} = 0, \quad (10)$$

where $C(x^1, x^2)$ is some constant (independent on $x_{(m)}^3$). Here the derivative over φ is taken assuming x^1 and x^2 constant (along the magnetic field line). We see that in the case of constant temperature, the last term of second part of Eq.(7) is zero.

The coordinates x^3 in neighboring LMCS are coupled by the following rule,

$$\frac{x_{(m)}^3 - \varphi_{max}^{(m)}}{S_{(m)}} = \frac{x_{(m+1)}^3 - \varphi_{min}^{(m+1)}}{S_{(m+1)}}. \quad (11)$$

It should be noted, we do not modify our “reference cut” used in Ref. [6] to build the coordinate system - it remains the surface $\varphi = const$.

Let us check here the properties of the new coordinates. Here we notate with x^i “old” local magnetic coordinates where x^1 and x^2 are magnetic coordinates which satisfy the magnetic differential equation (1) and coincide with local magnetic coordinates on the reference cut and $x^3 = \varphi$. “New” local magnetic coordinates will be denoted here with x_{new}^i . These coordinates differ only by the third coordinate, $x_{new}^1 = x^1$, $x_{new}^2 = x^2$ and x_{new}^3 is given by (8). It follows from (8) that

$$B_{new}^3 \equiv \mathbf{B} \cdot \nabla x_{new}^3 = \frac{\partial(x^1, x^2, x_{new}^3)}{\partial(x^1, x^2, \varphi)} B^{\varphi} = S_{(m)} (B)^2 \quad (12)$$

Therefore,

$$h_{new}^3 = \frac{B_{new}^3}{B} = S_{(m)} B. \quad (13)$$

Due to $\nabla \cdot \mathbf{B} = 0$ quantity $\sqrt{g_{new}} B_{new}^3$ is constant along the magnetic field lines. Therefore $\sqrt{g_{new}}$ scales as $(1/B)^2$ along the field lines, like in Boozer coordinates. Using (12) we obtain

$$\sqrt{g_{new}} = \sqrt{g} \frac{\partial(x^1, x^2, x^3)}{\partial(x_{new}^1, x_{new}^2, x_{new}^3)} = \sqrt{g} \frac{\partial(x^1, x^2, x^3)}{\partial(x^1, x^2, x_{new}^3)} = \frac{\sqrt{g} B^\varphi}{S_{(m)} (B)^2} \quad (14)$$

where the numerator in the last expression is constant on the field line. Thus it is sufficient to compute it on the reference cut,

$$\sqrt{g} B^\varphi = R \frac{\partial(R, Z, \varphi)}{\partial(x^1, x^2, x^3)} B^\varphi = \frac{\partial(R, Z, \varphi)}{\partial(x^1, x^2, \varphi)} \hat{B}_\varphi = \left[\frac{\partial(R, Z)}{\partial(x^1, x^2)} \hat{B}_\varphi \right]_{\varphi=\varphi_m} = \frac{S_{(m)}}{\lambda}, \quad (15)$$

where \hat{B}_φ is the physical φ -component of \mathbf{B} . We introduced a quantity λ which is independent on the coordinate x^3 as follows,

$$\lambda(x^1, x^2) = \left(\frac{\partial(R, Z)}{\partial(x^1, x^2)} \right)^{-1} \frac{S_{(m)}}{\hat{B}_\varphi}. \quad (16)$$

$$\text{Thus,} \quad \sqrt{g_{new}} = \frac{1}{\lambda(B)^2} \quad (17)$$

Since in the following we use only new coordinates, we omit subscript *new* everywhere.

3 Re-weighting of particles

To perform a Monte Carlo procedure for Eq.(2), u is expressed through the density of test particles, n_t , as follows,

$$u = w n_t, \quad w = \frac{1}{N_t} \int d^3 r u_0, \quad (18)$$

where w is the weight of a single test particle, N_t is a total number of test particles at the beginning of evolution, and u_0 is an initial distribution of u . The normal component of the flux density is represented as

$$F_n \equiv \frac{\mathbf{F} \cdot d\mathbf{S}}{dS} = w \frac{\Delta N}{dS \Delta t}, \quad (19)$$

where $d\mathbf{S}$ is an area element (dS its module), ΔN is number of test particles passing through this area element per time Δt . The sink term $-\nu u$ is modeled by removal of particle fraction $\nu \Delta t$ during the time step Δt . The source S_u is modeled by adding ΔN particles in the volume element $d^3 r$:

$$\Delta N = \frac{S_u d^3 r \Delta t}{w}. \quad (20)$$

If the total input flux (input power) through the boundary, P , is prescribed, the number of test particles added in the system per time step Δt is

$$N_{\text{add}} = \int dS \frac{\Delta N}{dS} = \frac{\Delta t}{w} \int dS F_n = \frac{\Delta t}{w} P. \quad (21)$$

Sometimes it is useful, to re-define the weights of the test particles in the MC procedure, (e.g., to adjust the time step of the random process to the local plasma and magnetic field parameters which place very different

restrictions on the time step near the inner boundary and near the wall). In this case, the unknown u is expressed through the new unknown \tilde{u} as follows,

$$u(\mathbf{r}) = \mu(\mathbf{r})\tilde{u}(\mathbf{r}), \quad (22)$$

where $\mu(\mathbf{r})$ is some scalar function of coordinates. We re-define the diffusion tensor, convection velocity and conditional sink rate as follows,

$$\tilde{\mathbf{D}} = \mu\mathbf{D}, \quad \tilde{\mathbf{V}} = \mu\mathbf{V} - \mathbf{D} \cdot \nabla\mu, \quad \tilde{\nu} = \mu\nu, \quad (23)$$

so that the right hand side of Eq. (2) preserves its form,

$$\mu \frac{\partial \tilde{u}}{\partial t} = \nabla \cdot (\tilde{\mathbf{D}} \cdot \nabla \tilde{u} - \tilde{\mathbf{V}} \tilde{u}) - \tilde{\nu} \tilde{u} + S_u, \quad (24)$$

and, in particular, the flux density preserves its value,

$$\mathbf{F} = -\mathbf{D} \cdot \nabla u + \mathbf{V}u = \tilde{\mathbf{F}} = -\tilde{\mathbf{D}} \cdot \nabla \tilde{u} + \tilde{\mathbf{V}} \tilde{u}. \quad (25)$$

Since we are interested only in the stationary solution, we replace the physical time t by the “iteration time” τ so that (24) takes the form

$$\frac{\partial \tilde{u}}{\partial \tau} = \nabla \cdot (\tilde{\mathbf{D}} \cdot \nabla \tilde{u} - \tilde{\mathbf{V}} \tilde{u}) - \tilde{\nu} \tilde{u} + S_u. \quad (26)$$

Since Eq. (26) is of the same form as Eq. (2), the Monte Carlo realization is similar,

$$\tilde{u} = \tilde{w} \tilde{n}_t, \quad \tilde{w} = \frac{1}{N_t} \int d^3r \tilde{u}_0. \quad (27)$$

In particular, the normal component of the flux density is given by

$$F_n = \tilde{F}_n \equiv \frac{\tilde{\mathbf{F}} \cdot d\mathbf{S}}{dS} = \tilde{w} \frac{\Delta N}{dS \Delta \tau}, \quad (28)$$

i.e. the number of test particles passing through the area element dS per “iteration time” interval $d\tau$, normalized by the area element, dS and multiplied by the new weight. The fraction of particles removed per “iteration time” interval $d\tau$ is $\tilde{\nu} \Delta \tau$, and the number of particles added to the volume element d^3r per “iteration time” interval $d\tau$ is

$$\Delta N = \frac{S_u d^3r \Delta \tau}{\tilde{w}}. \quad (29)$$

The number of test particles added to the system per “iteration” time step Δt in case of a prescribed input flux is

$$N_{\text{add}} = \int dS \frac{\Delta N}{dS} = \frac{\Delta \tau}{\tilde{w}} \int dS F_n = \frac{\Delta \tau}{\tilde{w}} P. \quad (30)$$

In curvilinear coordinates, test particles are described by a pseudo-scalar density, $\mathcal{N} = \sqrt{g} \tilde{n}_t$,

$$\frac{\partial \mathcal{N}}{\partial \tau} = \frac{\partial}{\partial x^i} \left[\frac{\partial}{\partial x^j} \tilde{D}^{ij} \mathcal{N} - \tilde{V}_c^i \mathcal{N} \right] - \tilde{\nu} \mathcal{N} + \mathcal{S}. \quad (31)$$

Here,

$$\mathcal{S} = \sqrt{g} S_u, \quad \tilde{V}_c^i = \tilde{V}^i + \frac{1}{\sqrt{g}} \frac{\partial}{\partial x^j} \sqrt{g} \tilde{D}^{ij} = \tilde{V}_{\perp c}^i + \tilde{V}_{\parallel c}^i. \quad (32)$$

In the last expression in (32), the terms containing $V_{\perp}^i = \mathbf{V}_{\perp e} \cdot \nabla x^i$ and D_{\perp}^{ij} were grouped in $\tilde{V}_{\perp c}^i$, while the terms with $V_{\parallel}^i = V_{\parallel e} h^i$ and D_{\parallel}^{ij} were grouped in $\tilde{V}_{\parallel c}^i$.

Let us introduce a particular form of the scaling factor μ which will serve two purposes:

- The parallel diffusion tensor component, $\tilde{D}_{\parallel}^{33}$, will be dependent on x^3 only through a dependence of plasma parameters, but not through the geometrical terms, namely, \sqrt{g} and h^3 . The parallel effective convection velocity component, $\tilde{V}_{\parallel c}^3$, will contain no derivatives of the geometrical terms, namely \sqrt{g} and h^3 , and have no terms with $D_{\parallel e}$ which depend on x^3 through the geometrical terms. This removes the limitation on the parallel step by the magnetic field scale in this direction;
- The parallel effective convection velocity will not contain the derivatives of the density, thus, reducing the influence of the statistical noise in this quantity on the Monte Carlo process.

Both of these conditions are satisfied by

$$\mu = \frac{c_0 n_e}{(B)^2}, \quad (33)$$

where c_0 is some constant which we are free to choose. Thus, using (13) and (17) we obtain

$$\tilde{D}_{\parallel}^{33} = c_0 n_e D_{\parallel} \lambda \sqrt{g} (h^3)^2 = c_0 n_e D_{\parallel} S_{(m)}^2 = \frac{2}{3} c_0 \kappa_{\parallel e} S_{(m)}^2, \quad (34)$$

where $S_{(m)}$ is independent on x^3 . For the effective parallel convection velocity using Eq. (23), Eq. (32) and

$$V_{\parallel e} = V_{\parallel} + \frac{D_{\parallel}}{n_e} \mathbf{h} \cdot \nabla n_e = V_{\parallel} + \frac{2\kappa_{\parallel e}}{3n_e^2} \mathbf{h} \cdot \nabla n_e, \quad (35)$$

where V_{\parallel} is the parallel velocity of density convection (see Ref. [1]), we have

$$\tilde{V}_{\parallel c}^3 = \mu V_{\parallel e} h^3 - D_{\parallel}^{33} \frac{\partial \mu}{\partial x^3} + \frac{1}{\sqrt{g}} \frac{\partial}{\partial x^3} \sqrt{g} \mu D_{\parallel}^{33} = \frac{c_0 S_{(m)}}{B} n_e V_{\parallel} + \frac{2}{3} c_0 S_{(m)}^2 \frac{\partial \kappa_{\parallel e}}{\partial x^3}. \quad (36)$$

Thus, in case of constant temperature along the magnetic field lines, the effective parallel convection velocity $\tilde{V}_{\parallel c}^3$ is proportional only to the parallel fluid velocity V_{\parallel} . Moreover, for the steady parallel plasma motion such that

$$\nabla \cdot V_{\parallel} n_e \mathbf{h} = \frac{1}{\sqrt{g}} \frac{\partial}{\partial x^3} \sqrt{g} V_{\parallel} n_e h^3 = (B)^2 \frac{\partial}{\partial x^3} \frac{S_{(m)}}{B} n_e V_{\parallel} = 0, \quad (37)$$

$\tilde{V}_{\parallel c}^3$ is obviously independent of x^3 .

4 Results for W7-X

Implementation of the new coordinate and re-weighting technique increases the efficiency of the code by about a factor of 100. Here, we present results for the W7-X magnetic geometry (without real limiters, an artificial boundary is set on the outer closed magnetic surface). The three equations (continuity and both energy equations) are implemented completely. The parallel momentum equation currently is implemented in test geometry only, the additional geometrical terms will be included later. However, no fundamental problems are expected from them.

We prescribe 10 eV for both temperatures and 10^{12} cm^{-3} for density at the outer edge of the plasma. On the inner boundary, we prescribe 100 eV for temperatures and 10^{13} cm^{-3} for density. The profiles are as expected: the electron temperature reflects the structure of the magnetic field better than the ion temperature and much better than the density because of their different parallel transport. Indeed, the electron temperature in the island is almost constant, the ion temperature has a noticeable gradient across the island and the density exhibits an even stronger gradient. The statistical noise in the density profile is stronger than in either temperature, because their larger parallel transport works like a smoothing filter. The same behaviour can be seen for all sections of the device. Again, the effect of the different parallel transport is emphasized.

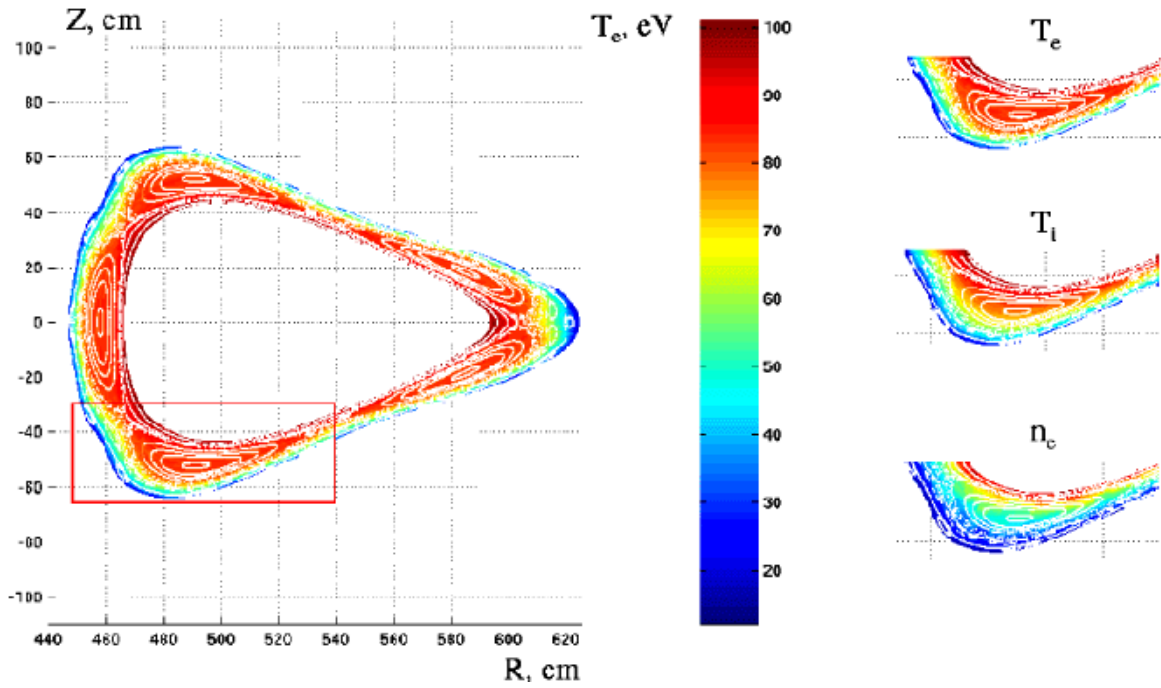


Fig. 1 Plasma parameter profiles of W7-X (real space).

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