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Benchmark of the 3-Dimensional Plasma Transport Codes E3D and BoRiS

A. Runov[a)], S. Kasilov[b)], J. Riemann[a)], M. Borchardt[a)], D. Reiter[c)], R. Schneider[a)]

[a)] Max-Planck Institut für Plasmaphysik, EURATOM Association, D-17491 Greifswald, Germany
[b)] Institut of Plasma Physics, National Science Center "Kharkov Institute of Physics and Technology", 61108, Kharkov, Ukraine
[c)] Institut für Plasmaphysik, Forschungszentrum Jülich GmbH, EURATOM Association, Trilateral Euregio Cluster, D-52425 Jülich, Germany
e-mail: runov@ipp.mpg.de

Abstract

The next generation of experiments - both for tokamaks and stellarators - requires the development of appropriate theoretical models. One important aspect here is the plasma edge physics description. Fluid transport codes extending beyond the standard 2-D code packages like B2-Eirene or UEDGE are under development. In the case of tokamaks, an interesting alternative line is the concept of an ergodic edge (necessary e.g. for ergodic divertors in TORE SUPRA or TEXTOR-94) creating a 3-D edge structure. To study these effects, a 3-D code E3D based upon a Multiple Coordinate Systems Approach is being developed. Presently, we are extending the program towards stellarator applications. A few new options are made available: single-island geometry and new formulation of boundary conditions.

For the new stellarator W7-X, a 3-D finite volume code BoRiS is being developed using magnetic (Boozer) coordinates. In this paper, we present a benchmark of both codes, for a test geometry (one single magnetic island in W7-X) including full 3-D metric variations, solving for the strongly anisotropic electron heat conduction equation.

1 Introduction.

E3D is a 3D scrape-off-layer (SOL) plasma transport code under development to solve a system of plasma fluid equations in a general magnetic geometry including intact magnetic surfaces, island chains and ergodic regions. It is a *fluid* Monte-Carlo code based upon our Multiple Coordinate System Approach (MCSA, see Ref. [1] for details). E3D was originally developed for tokamaks ergodic divertors (TEXTOR-94, TORE SUPRA) and is currently being extended towards stellarator applications (W7-X). In this paper we discuss new options: single-island geometry and a more accurate formulation of boundary conditions.

Another code (BoRiS, Ref. [2]) is also being developed to solve a system of plasma fluid equations, based upon a more conventional numerical approach (finite-volume discretization, like the well-known B2 code). BoRiS uses magnetic coordinates, thus allowing for standard discretization methods with higher order schemes retaining essential geometrical flexibility. It requires (for magnetic coordinates to exist) a negligible level of ergodicity.

Benchmarking of these two 3D codes based upon different numerical approaches against each other seems natural. The test model should be a compromise between

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geometrical complexity and physical transparence. Here, we have chosen an analytical representation (actually, a fit) for Boozer coordinates of a single island of the stellarator W7-X. Such a representation, which had been introduced in Ref. [3], was used in the present paper in a simplified form. We restrict ourselves to the conduction part of the electron energy equation, assuming constant plasma density.

In Section 2 we summarize the main ideas of MCSA and introduce the transport model equation used in both codes. In Section 3 we formulate a new approach to the boundary conditions, which is a non-trivial task for Monte-Carlo techniques in general coordinates. In Section 4, we describe the geometry of the test case (single island of W7-X) and discuss the results.

2 Transport model.

Let us consider the heat balance equation for electrons in the following vector form of the conservation law neglecting convection for simplicity,

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

Here T stands for the electron temperature, n is the plasma density (further assumed to be constant for simplicity), $\mathbf{h} = \mathbf{B}/B$ 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,

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

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, $\chi_\perp \equiv \kappa_\perp/n$ 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 [4]). For such a coordinate system, the minimum requirement is that the first two variables x^i must satisfy the magnetic differential equation,

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

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 $\mathbf{e}_3$ points 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 neighbouring coordinate systems with the help of an Interpolated Cell Mapping technique (a precomputed transformation of lines $x^1 = const.$ and $x^2 = const.$, interpolated by means of bicubic splines). By increasing the mesh size 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-parametrical families of curves on some surface which is never tangential to the magnetic field. In [1] we used a 2D Cartesian mesh for this purpose. In the particular case when Boozer coordinates (s, ϑ, φ) are available everywhere in computational region, the coordinate lines can be used as the base curves (initial conditions for Eq. (4)). One can build the local magnetic coordinates x^i as follows:

$$x^1 = s, \qquad x^2 = \vartheta - \iota\varphi, \qquad x^3 = \varphi. \tag{6}$$

3 Boundary conditions.

Using a set of local coordinate systems, we have already made our choice of numerics in favour of Monte-Carlo. Indeed, an individual fluid "parcel" retains its identity also when it is handed over from one coordinate system to a neighbouring one. This avoids the otherwise arising problem of numerical diffusion. Within a single local coordinate system, our approach reduces to a conventional Monte-Carlo method for convection-conduction equations in curvilinear coordinates.

There are three commonly used kinds of boundary conditions to Eq. (1): 1) prescribed value T on a boundary; 2) prescribed incoming flux through a boundary; 3) prescribed relation between the value on and outgoing flux through a boundary (frequently formulated as a given decay length). The Monte-Carlo realization of the first two problems is rather straightforward. Indeed, we know the statistical weight of a parcel, thus, in the case (1) we have to sustain a given amount of parcels in all boundary cells (eventually taking account of the gradient of T in the distribution of parcels). In the second case, we have e.g. to reflect the "old" parcels from the boundary and to keep a source of the "new" parcels of known intensity through the boundary.

The third kind of boundary condition (conditional sink of parcels) is more complicated: it should be formulated in terms of the probability A of the absorbtion of the parcels. Let us first derive A in the 1D case to demonstrate the basic principle. In the vicinity of the boundary we can neglect the gradient of T and convection. We have to keep the condition $\Gamma = wV_n$, where Γ physically means the outgoing flux, $w = 1.5nT$ and V_n is a preset normal component of velocity. The 1D equation obtained is of the form

$$\frac{\partial w}{\partial t} = \chi \frac{\partial^2}{\partial x^2} w. \tag{7}$$

The corresponding random walk process with Gaussian distribution of random numbers can be described with an integral operator as follows:

$$w(x) = \int_{-\infty}^{\infty} dx' P(x - x') w_0(x'), \quad \text{where} \quad w_0(x') = const, \tag{8}$$

$$\text{and} \qquad P(\Delta x) = \frac{1}{\sqrt{4\pi\chi\Delta t}} \exp\left(-\frac{\Delta x^2}{4\chi\Delta t}\right). \tag{9}$$

After the time step Δt the total weight of the particles crossing the wall ($x = 0$) is

$$\Delta W = \int_{-\infty}^{0} dx w(x) = w_0 \int_{-\infty}^{0} dx \int_{0}^{\infty} dx' P(x - x') = w_0 \sqrt{\frac{\chi\Delta t}{\pi}}. \tag{10}$$

On the other hand, the boundary condition states that this weight must be

$$\Delta W_{out} = w_0 V_n \Delta t = A \Delta W, \quad \text{hence} \quad A = \sqrt{\frac{\pi V_n^2 \Delta t}{\chi}}. \tag{11}$$

In 3D, we introduce an additional Cartesian coordinate system (x, y, z), z taken along the magnetic field line. Let us remember that any linear combination of Gaussian random numbers also obeys a Gaussian distribution. Thus, if we perform our step in general coordinates x^1, x^2, x^3 with Gaussian random numbers, we will obtain for x, y, z the following transition probability:

$$P(\Delta x, \Delta y, \Delta z) = \frac{1}{4\pi\chi_\perp\sqrt{4\pi\chi_\parallel}} \exp\left(-\frac{\Delta x^2 + \Delta y^2}{4\chi_\perp\Delta t} - \frac{\Delta z^2}{4\chi_\parallel\Delta t}\right). \tag{12}$$

As in the 1D case, we need the total weight ΔW, which crosses a unit square element of the wall in time Δt. Let us introduce the rotated coordinate system x_1, y_1, z_1, where the axis x_1 is normal to the wall. Then

$$\Delta W = w_0 \int_{-\infty}^{0} dx_1 \int_{0}^{\infty} dx_1' \int_{-\infty}^{\infty} dy_1 \int_{-\infty}^{\infty} dz_1 P_1(x_1 - x_1', y_1 - y_1', z_1 - z_1'), \tag{13}$$

where we use the probability distribution from Eq. (12) and take into account the rotation of the coordinate system. The result of the integration is

$$\Delta W = w_0 \sqrt{\frac{(\chi_\parallel \sin^2\alpha + \chi_\perp \cos^2\alpha)\Delta t}{\pi}}, \tag{14}$$

where α is the angle between the field line and the wall. This weight must be equal to $V_n \Delta t w_0 / A$, thus, for the absorbtion coefficient, we have

$$A = \sqrt{\frac{\pi V_n^2 \Delta t}{\chi_\parallel \sin^2\alpha + \chi_\perp \cos^2\alpha}}. \tag{15}$$

4 Test geometry and results.

In the present paper we test our numerical realization of the magnetic field geometry and of boundary conditions (mixed condition). To that effect, we need a benchmark

case to compare our solutions properly. Here, we base our treatment upon the analytical formulas of Ref. [3] for Boozer coordinates of a single island of the stellarator W7-X. The fit formulae obtained in Ref. [3] for a single island through the chain of the codes GOURDON → DESCUR → VMEC → JMC are:

$$\begin{aligned} \sqrt{g} &= -534. - 86.\cos(2\pi\varphi), \qquad g_{s\vartheta} = 5.6\sin[4\pi(\vartheta-\varphi)] && (16)\\ g^{ss} &= s(43. + 37.\cos[4\pi(\vartheta-\varphi)]) && (17)\\ F'_T &= \pi, \quad I = 882, \quad \iota \equiv F'_P/F'_T = 1.085, && (18) \end{aligned}$$

together with usual "plasma edge approximation" $J = 0$, $g^{\varphi s} = 0$. Here, F_T and F_P are toroidal and poloidal magnetic fluxes, respectively, J and I are toroidal and poloidal currents, respectively, ι is the rotational transform. This information is sufficient to derive the full metric tensor of Boozer coordinates,

$$\begin{aligned} B_0^2 &= -\frac{IF'_T}{\sqrt{g}} \qquad\qquad g_{\vartheta\vartheta} = \frac{1}{B_0^2}F'^2_T g^{ss} && (19)\\ g_{\vartheta\varphi} &= -\frac{1}{B_0^2}F'_T F'_P g^{ss} \qquad g_{\varphi\varphi} = \frac{1}{B_0^2}\left(I^2 + F'^2_P g^{ss}\right) \end{aligned}$$

For our test purposes, this model geometry of an island can be simplified further. We neglect the angular dependence of $\sqrt{g}$ and set $\iota = 1$ (here, we induce an error of about 15%).

Taking account of Eqs. (16), (19) and the transformation rule (6), we obtain the contravariant metric tensor of our local magnetic coordinate system:

$$\begin{aligned} g^{11} &= g^{ss}, \quad g^{12} = g^{s\vartheta}, \quad g^{13} = 0\\ g^{22} &= g^{\vartheta\vartheta} - \iota g^{\vartheta\varphi}, \quad g^{23} = 0, \quad g^{33} = g^{\varphi\varphi} \qquad (20)\\ h^3 &= h^\varphi = \sqrt{\frac{F'_T}{-I\sqrt{g}}}. \end{aligned}$$

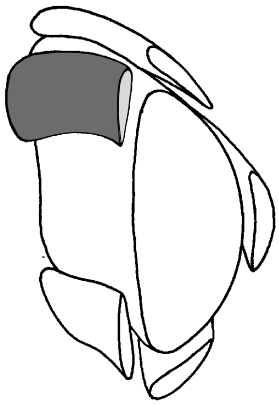

Fig. 1: Benchmark geometry: Single island (real space).

It is easy to see that in the (artificial) case of no dependence of $\chi_\parallel$ on the temperature, one can separate the variables in Eq.(2) and reduce the dimensionality of the problem by 1 (the additional requirement here is the symmetry of the boundary conditions along x^3). It seems reasonable to define $\chi_\parallel(T) \equiv \chi_\parallel(T_0)$ for some fixed temperature T_0 and to use the simplified equation as the test transport model. The resulting (steady-state) 2D equation

$$\frac{\partial}{\partial x^1}\left(g^{11}\frac{\partial T}{\partial x^1} + g^{12}\frac{\partial T}{\partial x^2}\right) + \frac{\partial}{\partial x^2}\left(g^{21}\frac{\partial T}{\partial x^1} + g^{22}\frac{\partial T}{\partial x^2}\right) = 0 \qquad (21)$$

can be solved both with E3D and BoRiS. Moreover, there exist pre-packaged library subroutines able to solve such a problem. In the present work, we use the D03RAF subroutine from the NAG library as an additional check of the results.

The computational domain for the test calculations corresponds approximately to the single island of W7-X described above (Fig.1 shows the island in real space). For

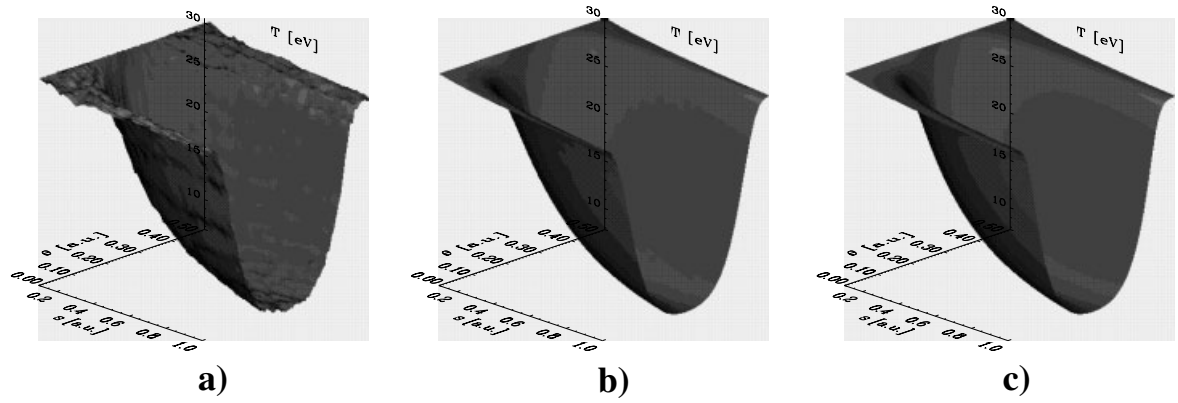

Fig. 2: The solution of the Eq. (21) by means of E3D (a), BoRiS (b) and D03RAF (c) .

purposes of this the test, we impose an artificial "inner" boundary at $s = 0.1$ (just a hole in the middle of the island) and fix the temperature to 30eV there. On the "outer" boundary ($s = 1$), we preset the following relation between the temperature and the outgoing heat flux:

$$q \equiv g^{11}\frac{\partial T}{\partial x^1} + g^{12}\frac{\partial T}{\partial x^2} = \sqrt{g^{11}}\gamma T, \qquad \text{where} \qquad \gamma = 0.0555.$$

The results of modelling with all three methods are presented in Fig.2. They demonstrate very good agreement within the numerical accuracy. The steep gradient in the profile of T is a pure geometrical effect (the island is very strongly elongated in real space, see Fig.1).

5 Conclusions

A new formulation of the boundary conditions for the code E3D has been developed and built in as a regular option. A simplified magnetic geometry which allows the non-trivial benchmarking of the plasma transport codes has been proposed. The results obtained with both E3D and BoRiS codes demonstrate a good agreement with each other and with the "sample" solution from D03RAF subroutine (NAG library).

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