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W7-X edge modelling with the 3D SOL fluid code BoRiS

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Abstract

BoRiS is a 3D scrape-off layer (SOL) transport code under development which is to solve a system of plasma fluid equations. BoRiS is currently extended towards a physics model including continuity, parallel momentum and energy equations for both electrons and ions. In addition the code requires the implementation of adequate solvers and the generation of high precision metric coefficients throughout the entire computational domain. © 2001 Published by Elsevier Science B.V.

Keywords: Island divertor; Stellarator; Edge modelling

1. Introduction

BoRiS is a new 3D scrape-off layer (SOL) transport code aimed at solving a system of plasma fluid equations like the well-known B2 code. In order to deal with the complex 3D geometry of W7-X, BoRiS uses magnetic coordinates, thus allowing for standard discretization methods with higher order schemes retaining full geometric flexibility. Serving as a test bed for the overall layout of BoRiS a system of two coupled anisotropic Laplace equations for the electron and ion temperature was implemented in a first step. Fig. 1 shows one period of a W7-X plasma in real space with the colours indicating the electron temperature profiles on the outermost flux surfaces of the magnetic island flux tubes. Subsequently the actual physics model of BoRiS has been extended by including equations for both the parallel velocity and the plasma density. Parallel to this work numerical aspects like the implementation of more sophisticated solvers, problems arising from grid generation and the generation of high precision metric information are covered as well.

2. Model equations

Having started with a system of simplified energy equations [1,2] for the electrons and ions consisting of two anisotropic Laplace equations being coupled by a heat exchange term, the actual physics model of BoRiS is currently completed by including the equations for the parallel momentum and the plasma density, leading to the following system:

$$\begin{aligned}
&\vec{\nabla}_{\parallel}(n_i\vec{u}_{\parallel}) - \vec{\nabla}_{\perp}(D_{\perp}\vec{\nabla}_{\perp}n_i) = S_n^i,\\
&\vec{\nabla}_{\parallel}(m_i n_i u_{\parallel}^2) - \vec{\nabla}_{\perp}(m_i\vec{u}_{\parallel}D_{\perp}\vec{\nabla}_{\perp}n_i)\\
&\quad = -\vec{\nabla}_{\parallel}(p_e + p_i - \eta_{\parallel}\vec{\nabla}_{\parallel}\vec{u}_{\parallel}), \qquad (1)\\
&\vec{\nabla}_{\parallel}\left(\frac{5}{2}T_a n_i\vec{u}_{\parallel} - \kappa_{\parallel}^a\vec{\nabla}_{\parallel}T_a\right)\\
&\qquad + \vec{\nabla}_{\perp}\left(-\frac{5}{2}T_a D_{\perp}\vec{\nabla}_{\perp}n_i - \kappa_{\perp}^a\vec{\nabla}_{\perp}T_a\right)\\
&\quad = \operatorname{sgn} a(\vec{u}_{\parallel}\vec{\nabla}_{\parallel}p_e - Q_{ei}), \qquad (2)
\end{aligned}$$

where a stands for electrons e and ions i with $\operatorname{sgn} e = -\operatorname{sgn} i = -1$. Here we have the ion density $n_i = n_e = n/2$, the parallel velocity $u_{\parallel}$ (with $\vec{u} = \vec{u}_{\parallel} + \vec{u}_{\perp} = \vec{u}_{\parallel} - D_{\perp}\vec{\nabla}_{\perp}n_i/n_i$), the temperatures T_a, the parallel and perpendicular conductivities $\kappa_{\parallel}^a$ and $\kappa_{\perp}^a$, an anomalous diffusivity $D_{\perp}$, the heat exchange term Q_{ei} and a source term S_{n_i}. Although the above equations correspond to the stationary case, artificial time dependencies are taken into account for numerical stability reasons.

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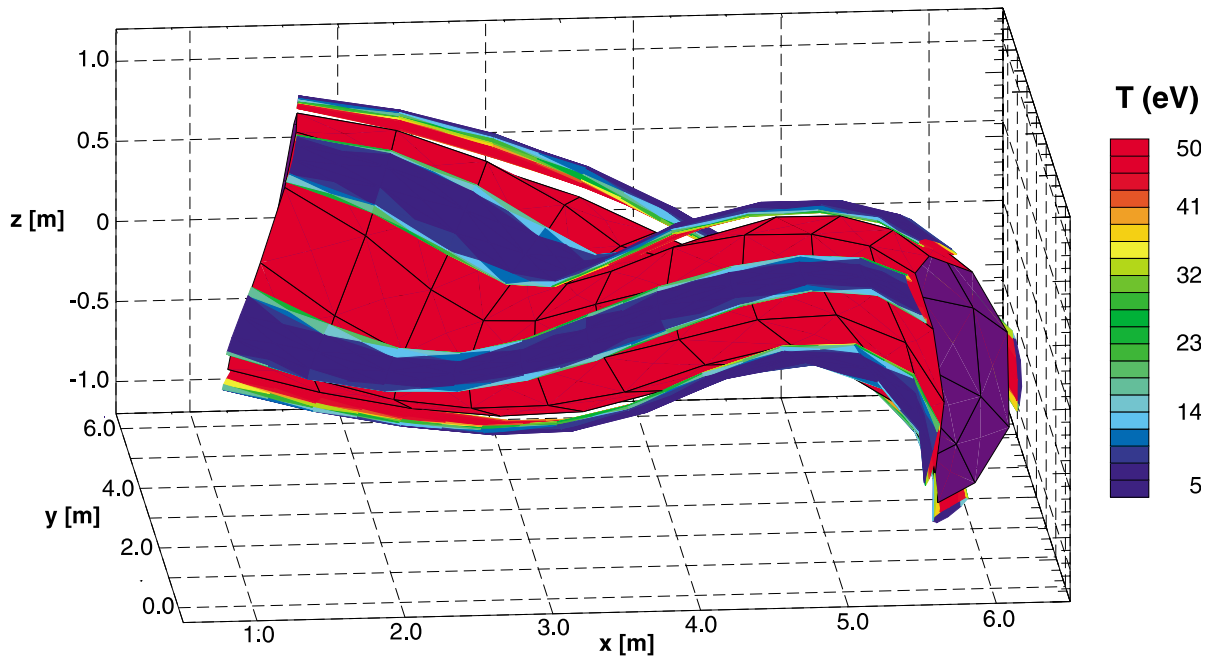

Fig. 1. Island flux tubes with electron temperature profiles in real space.

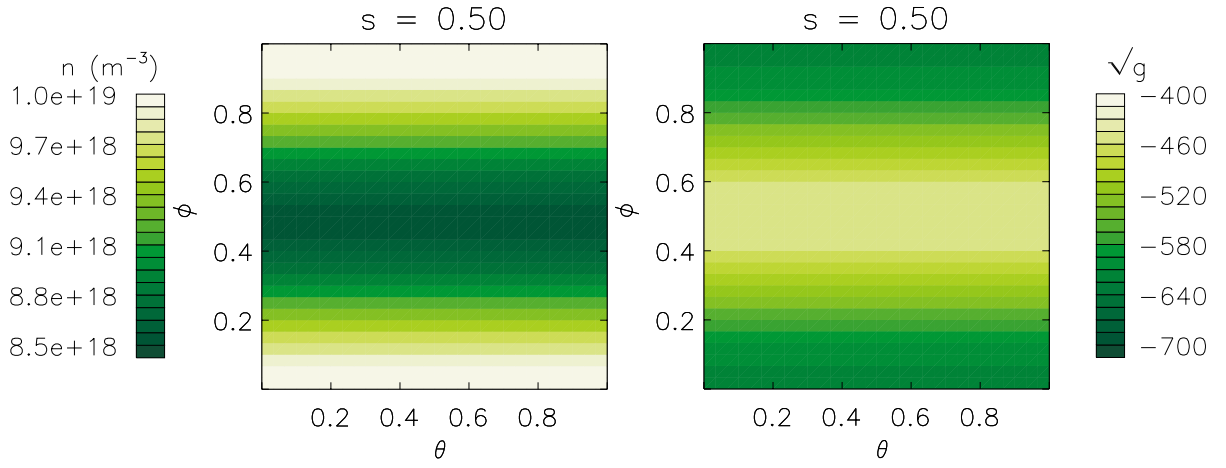

Fig. 2. Density profile (left) and metric coefficient $\sqrt{g}$ (right).

3. Continuity equation tests

In implementing the new equations, we performed several tests in different geometries. A simple slab model can be used to test basic properties and different contributions. On the other hand, the equations can also be solved serving as a diagnostic tool for the specifics of the actual 3D geometry.

As an example, the continuity equation was solved in a W7-X geometry assuming the absence of sources and a spatially constant test-velocity field $\vec{u} = (u_{\parallel}, u_{\perp 1}, u_{\perp 2})$. Using different components of the test-velocity, the metric properties of the computational domain were probed, thus yielding a fingerprint of the geometry.

Fig. 2 shows the density profile $n(s = \text{const})$ as obtained with a velocity field $\vec{u} = (u_{\parallel}, 0, 0)$ in comparison to the metric coefficient $\sqrt{g}$ which acts as a weight factor on the interfaces between computational cells. Since $\vec{u}$ is parallel to the magnetic field there is only a 1D variation along the toroidal coordinate ϕ.

Fig. 3 compares two results for the density (upper and lower) to the metric coefficient g^{ss} (middle). The

upper case corresponds to $\vec{u} = (u_{\parallel}, 0, u_{\perp 2})$ and shows the same characteristic pattern as g^{ss} together with a toroidal background variation that can be related to the action of $\sqrt{g}$ according to Fig. 2. This test-velocity is 2D as it lies completely within a magnetic flux surface and therefore does not yield a radial variation of the density profiles. Such variation of the density as it is predicted by g^{ss} can only be detected if a velocity component along the s direction is introduced as was done in the lower case where $\vec{u} = (0, u_{\perp 1}, 0)$. Again, the characteristic pattern due to g^{ss} and a toroidal variation can be seen.

4. Interpolation of scattered 3D data

As already outlined earlier [2], BoRiS utilizes a physically motivated scheme of interpolation which yields the value f_* of a function and its partial derivatives at $\vec{r}_*$ as weighted averages from neighbour grid point values f_i

$$f_* = \frac{1}{W}\sum_{i=1}^{N} w_i f_i, \quad W = \sum_{i=1}^{N} w_i. \tag{3}$$

The weight factors w_i are

$$w_i = \gamma(P_{i*}) \exp\left(-|\vec{r}_i - \vec{r}_*|^2/\lambda_*^2\right), \tag{4}$$

where λ_* denotes a local grid constant which acts as a local 'screening length' for the properties of surrounding grid points determining the value at $\vec{r}_*$. The partial derivatives of f with respect to the elementary directions $\vec{e}_j$ are

$$\left.\frac{\partial f}{\partial x^j}\right|_* = \lim_{\epsilon \to 0} \frac{1}{W^j}\sum_{i=1}^{N} w_i^j (x_i^j - x_*^j)\frac{(f_i - f_*)}{(x_i^j - x_*^j)^2 + \epsilon},$$
$$W^j = \sum_{i=1}^{N} w_i^j. \tag{5}$$

Here the weight factors w_i^j are

$$w_i^j = w_i \cos^2 \alpha_{i*}^j, \tag{6}$$

with α_{i*}^j being the angle between $\vec{r}_{i*}$ and $\vec{e}_j$. The factor γ in (4) provides a possible *upwind* correction [3] to the individual weight w_i due to the presence of a carrier field in a general convection-diffusion situation

$$\gamma(P_{i*}) = (e^{P_{i*}/2} - 1)/(e^{P_{i*}} - 1). \tag{7}$$

This factor appears as though the interface position $\vec{r}_*$ was central to the surrounding grid points $\vec{r}_i$. In this approach spatial asymmetries are taken care of by the second factor in (4). The dimensionless number P_{i*} is the projection of the local Péclet number which measures convection versus diffusion strength for each equation individually. Using more or less simple approximations to the function (7) different schemes of interpolation are available (e.g. *upwind*, *hybrid*, *power law* [3]).

5. Numerical issues

To solve the above system of nonlinear equations (1) with a Newton method the implementation of sophisticated solvers is crucial to the spatial resolution available. BoRiS is designed to utilize several solvers based on different methods [4]:

(i) sparse direct solver – MA28 [5];
(ii) sparse iterative solver – BiCGSTAB or GMRES(m) with left and right preconditioning (Jacobi, SGS, SOR, SSOR, ILU(0), ILUT(p, τ));
(iii) matrix-free iterative solver – BiCGSTAB or *GMRES(m)* with Jacobi preconditioning.

Currently the best results are obtained with sparse iterative solvers and an ILU(0) preconditioning. However, this method is still rather time-consuming and memory-expensive and will be replaced by an adequate matrix-free solver. The memory requirements for the different solvers can be compared as

$$\frac{\text{direct solver}}{\text{iterative solver}} \approx 300$$

and

$$\frac{\text{iterative solver}}{\text{matrix-free solver}} \approx 25.$$

In addition to appropriate solvers, local grid refinement offers a maximum of spatial resolution where it is necessary while minimizing the numerical effort for solving the problem. In a future version BoRiS will use an adaptive apparatus for grid generation and refinement. At the present stage, first tests were performed resolving a pre-defined region of the computational domain to a higher degree than its surroundings, showing satisfactory results.

6. Magnetic coordinates

Lastly, the solution of the 3D transport equations in magnetic coordinates requires good knowledge of the spatially-varying metric coefficients, in particular near the island chain boundary in the W7-X edge that BoRiS must resolve. The current MHD codes do not appropriately treat such separatrix regions when computing metric coefficients, thus we have developed a new method for their evaluation. This method assumes only the existence of magnetic surfaces (so zero ergodicity) and knowledge of the magnetic field (and its derivatives) in the region of interest. We first identify the X- and O-points of the field by finding where the field lines close upon themselves after only one toroidal turn. Then, for each topological region (plasma core, islands, SOL), we

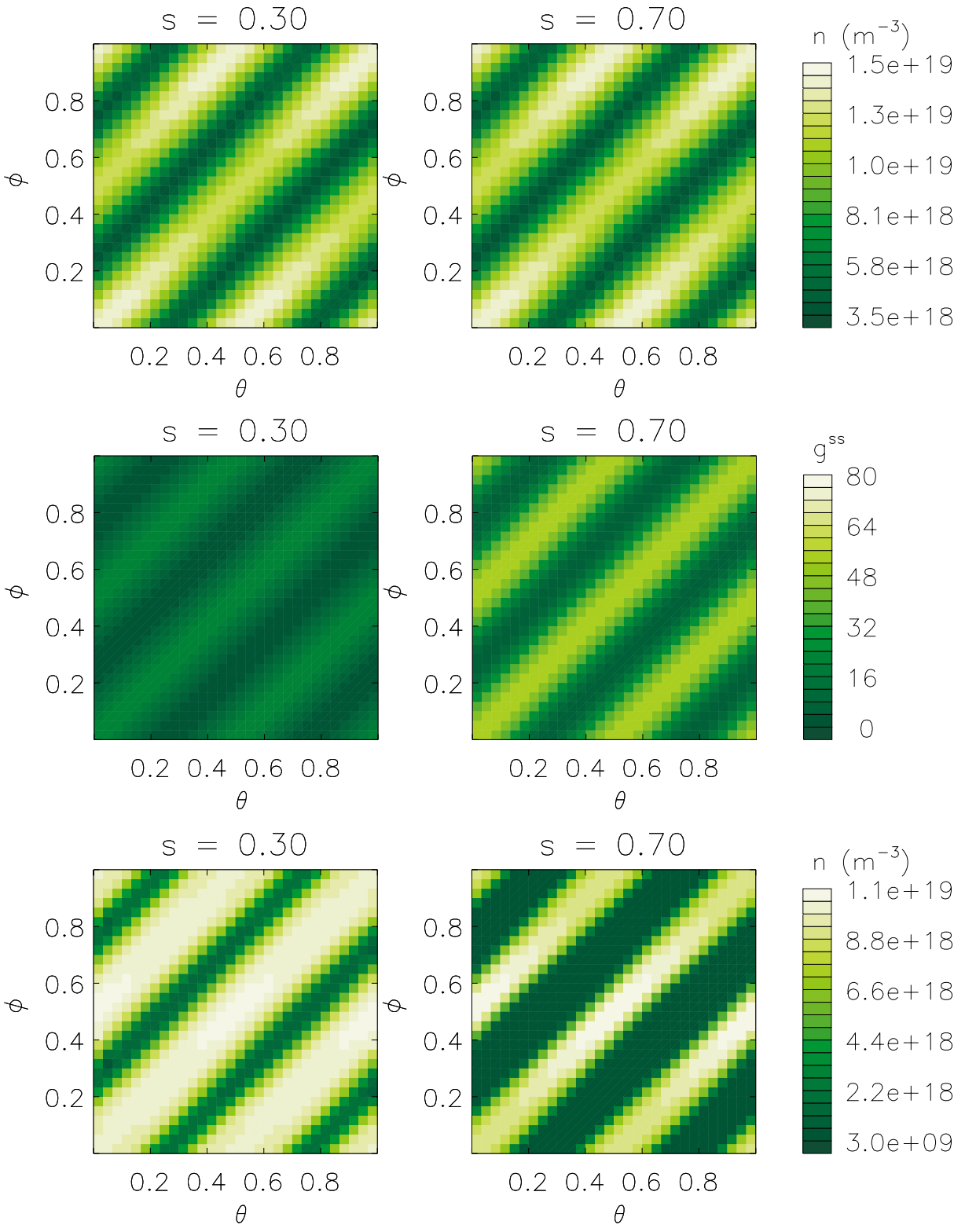

Fig. 3. Density profiles (upper and lower) and metric coefficient g^{ss} (middle).

follow field lines long enough to describe the magnetic surfaces to the desired accuracy (i.e., a few hundred toroidal turns). On these surfaces, we can now compute the rotational transform ι, the toroidal flux F_T, and the poloidal and toroidal currents I and J. To proceed further, we make use of an algorithm developed by Nemov [6] which allows one to recast magnetic differential equations of the form $\vec{B} \cdot \nabla f = 0$ as initial value problems necessitating only integration along the field lines. By so doing, we can obtain numerical expressions for the Clebsch components of the field $\nabla\psi$ and $\nabla(\theta - \iota\zeta)$ in each plasma region. The metric coefficients are then trivially obtained. The determination of the Nemov initial conditions requires the radial derivative $\partial F_T/\partial R$, which is the only radial derivative appearing. Moreover, all integrations are done along field lines, allowing this method to provide the desired numerical accuracy for our purposes.

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