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A novel flexible field-aligned coordinate system for tokamak edge plasma simulation

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ABSTRACT

Tokamak plasmas are confined by a magnetic field that limits the particle and heat transport perpendicular to the field. Parallel to the field the ionised particles can move freely, so to obtain confinement the field lines are "closed" (i.e. form closed surfaces of constant poloidal flux) in the core of a tokamak. Towards, the edge, however, the field lines intersect physical surfaces, leading to interaction between neutral and ionised particles, and the potential melting of the material surface. Simulation of this interaction is important for predicting the performance and lifetime of future tokamak devices such as ITER. Field-aligned coordinates are commonly used in the simulation of tokamak plasmas due to the geometry and magnetic topology of the system. However, these coordinates are limited in the geometry they allow in the poloidal plane due to orthogonality requirements. A novel 3D coordinate system is proposed herein that relaxes this constraint so that any arbitrary, smoothly varying geometry can be matched in the poloidal plane while maintaining a field-aligned coordinate. This system is implemented in BOUT++ and tested for accuracy using the method of manufactured solutions. A MAST edge cross-section is simulated using a fluid plasma model and the results show expected behaviour for density, temperature, and velocity. Finally, simulations of an isolated divertor leg are conducted with and without neutrals to demonstrate the ion-neutral interaction near the divertor plate and the corresponding beneficial decrease in plasma temperature.

1. Introduction

The plasma in the core of a tokamak is confined by magnetic fields that do not intersect any physical surfaces, but instead twist endlessly to form closed surfaces of poloidal flux. The separatrix marks the dividing line between these "closed" field lines and ones that are "open" (i.e. ones that intersect the walls of the tokamak). These open field lines are designed to intersect the divertor, which is made to withstand the particle and heat flux that escapes the core of today's machines. In future devices such as ITER, however, the power flux could potentially be too high (>10 MW/m^2) for any known material to withstand for prolonged periods of time [1]. By injecting neutral gas into the divertor region the plasma can be driven into a detached regime where the majority of the plasma power is radiated away before the plasma reaches the divertor, significantly lowering the plasma power deposited on it. It is essential to accurately simulate such detached plasmas to predict the heat loads that will remain for these larger future devices [2]. For this, it is important to match the simulation grid to the geometry of the divertor, which many codes currently do in the 2D poloidal plane, but the 3D extent remains unoptimised to the tokamak geometry due to the field-aligned nature of the plasma perturbations.

In tokamak plasmas, waves and instabilities are elongated along the magnetic field, while the perpendicular structures are small (on the order of the Larmor radius). Therefore, when simulating an edge plasma it is desirable to also have a coordinate system and grid that are aligned along the field. One can derive a set of coordinates related to standard orthogonal tokamak coordinates (ψ, θ, ϕ as shown in Fig. 1) where one coordinate is aligned to the field. Such a coordinate system allows for resolution along the field line to be sparser as is appropriate for the large structures, while maintaining fine resolution perpendicular to the magnetic field. The typical method for doing this is to keep the radial flux coordinate ψ, but to replace the toroidal angle ϕ and the poloidal angle θ with a shifted toroidal angle z and field-aligned coordinate y, respectively [3,4]. The mathematical derivation of this is detailed in the next section, but qualitatively this implies that if ψ and z are held constant while y is increased, one will progress along the field line on a helical path around the torus. The toroidal angle changes as one moves in y, implying that these coordinates are no longer orthogonal.

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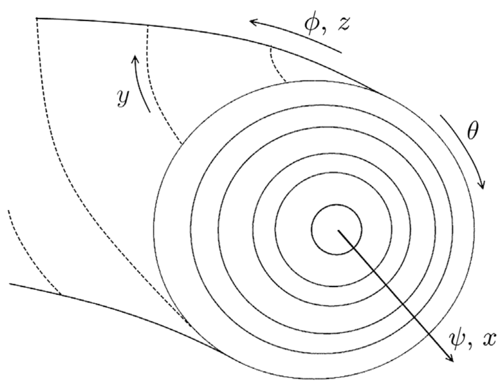

Fig. 1. The geometry described by the coordinate system posed in Eq. (1).

Though this system solves the problem of resolution, it leaves other problems un-addressed. Namely, the grid is restricted in shape in the poloidal plane because the ψ coordinate is orthogonal to the poloidal projection of y. If this constraint is lifted by deriving a new set of coordinates that are both field-aligned but also non-orthogonal in ψ and y, there is freedom to define a grid that matches the geometry of a specific tokamak in the divertor region. This is especially useful for the simulation of neutrals because they do not follow the field, so a wall-conforming grid is necessary. In this paper, a novel coordinate system that allows such freedom is presented, tested, and utilised for divertor plasma simulations.

An important distinction needs to be made between this new system and current coordinate systems in use in plasma edge codes such as SOLPS [5] and EDGE-2D [6]. These codes are 2D, so though they do allow non-orthogonality in the poloidal grid, they do not have a field-aligned coordinate. The coordinate system derived in this paper allows for 3D plasma edge simulation grids to be defined with non-orthogonalities in the poloidal plane while also maintaining a field-aligned coordinate.

1.1. Standard field-aligned coordinates

In the derivation of these coordinates, standard symbols for tokamak geometry are utilised for the toroidal, poloidal, and radial flux coordinates—ϕ, θ, and ψ respectively [7]. These coordinates form a right-handed, orthogonal coordinate system as shown in Fig. 1. The standard field-aligned coordinate system is defined as

$$\begin{aligned} x &= \psi \\ y &= \theta \\ z &= \phi - \int_{\theta_0}^{\theta} \nu \, d\theta \end{aligned} \tag{1}$$

where the local field line pitch is given by

$$\nu(\psi,\theta) = \frac{\partial\phi}{\partial\theta} = \frac{\mathbf{B}\cdot\nabla\phi}{\mathbf{B}\cdot\nabla\theta} = \frac{B_\phi h_\theta}{B_\theta R}. \tag{2}$$

with toroidal field B_ϕ, poloidal field B_θ, major radius R, and poloidal arc-length h_θ. Fig. 1 shows the geometry described by the coordinate system in Eq. (1). It is important to notice that the shift added to the z-coordinate causes the y-coordinate to be field-aligned. The x-coordinate remains perpendicular to the poloidal projection of the y-coordinate, limiting choice of poloidal geometry.

The contravariant basis vectors are then found by taking the gradient of each coordinate, using $\nabla = \nabla\psi\frac{\partial}{\partial\psi} + \nabla\theta\frac{\partial}{\partial\theta} + \nabla\phi\frac{\partial}{\partial\phi}$ to calculate

$$\begin{aligned} \nabla x &= \nabla\psi \\ \nabla y &= \nabla\theta \\ \nabla z &= \nabla\phi - \nu\nabla\theta - I\nabla\psi \end{aligned} \tag{3}$$

with

$$I = \int_{\theta_0}^{\theta} \frac{\partial\nu}{\partial\psi}\, d\theta. \tag{4}$$

The magnetic field can be written in Clebsh form [8],

$$\mathbf{B} = \nabla x \times \nabla z = \frac{1}{\mathbf{J}}\mathbf{e}_y \tag{5}$$

so the coordinate system is field aligned. The contravariant and covariant metric tensors are defined as

$$\begin{aligned} g^{ij} &= \nabla u^i \cdot \nabla u^j \\ g_{ij} &= \mathbf{e}_i \cdot \mathbf{e}_j \end{aligned} \tag{6}$$

where $\mathbf{e}_i = \mathbf{J}(\nabla u^j \times \nabla u^k)$ and u^i indicates a particular coordinate. Using the following identities

$$\nabla\psi = R\,|B_\theta| \quad \nabla\theta = |h_\theta|^{-1} \quad \nabla\phi = R^{-1} \tag{7}$$

the contravariant metric tensor can be rewritten as

$$g^{ij} = \begin{bmatrix} (RB_\theta)^2 & 0 & -I(RB_\theta)^2 \\ \cdots & h_\theta^{-2} & \nu h_\theta^{-2} \\ \cdots & \cdots & I^2(RB_\theta)^2 + \nu^2 h_\theta^{-2} + R^{-2} \end{bmatrix}. \tag{8}$$

To calculate the covariant metric tensor, one must first find the Jacobian of the system, which is given by

$$\mathbf{J}^{-1} = \nabla x \cdot (\nabla y \times \nabla z) \tag{9}$$

thus

$$\mathbf{J} = \frac{h_\theta}{B_\theta}. \tag{10}$$

The covariant metric tensor, defined as g_{ij} in Eq. (6), is then calculated as

$$g_{ij} = \begin{bmatrix} I^2R^2 + (RB_\theta)^{-2} & B_\phi h_\theta I R B_\theta^{-1} & IR^2 \\ \cdots & h_\theta^2 + R^2\nu^2 & \nu R^2 \\ \cdots & \cdots & R^2 \end{bmatrix}. \tag{11}$$

These co- and contravariant metric tensors can be used within simulations to perform operations, such as the parallel gradient, $\nabla_\parallel = \hat{b}\cdot\nabla = \frac{1}{\boldsymbol{J}\boldsymbol{B}}\frac{\partial}{\partial y}$, in the correct geometry [4]. It is important to note that there is a singularity in this coordinate system wherever $B_\theta = 0$ ($\boldsymbol{J} \to \infty$ in Eq. (9)), such as at the X-point. The new and improved coordinate system described in the next section still contains this same limitation.

2. Flexible field-aligned coordinates

Near the divertor, this standard field-aligned system suffers from the inability to match the physical geometry of the divertor surface due to the orthogonality constraint in the poloidal direction. Fig. 2 shows a line of constant θ, which represents a grid in the standard field-aligned coordinates. It is desirable to shift this line so that it lies on the divertor plate, which requires a shift in the θ coordinate. Though such a coordinate system is already utilised in many plasma codes for 2D simulations, a new set of coordinates is needed to allow a 3D simulation mesh to be aligned the divertor (or any smoothly varying) geometry in the poloidal plane while also maintaining field-alignment. To derive these coordinates, the following system is defined by analogue to Eq. (1):

$$\begin{aligned} x &= \psi \\ y &= \theta - y_{\text{shift}} \\ z &= \phi - z_{\text{shift}} \end{aligned} \tag{12}$$

such that the shift in y (y_{shift}) allows for the x-coordinate to be aligned with any arbitrary geometry in the poloidal plane. Likewise the shift in z (z_{shift}) enables the y-coordinate to follow an arbitrary

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