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# The field line map approach for simulations of magnetically confined plasmas



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#### ABSTRACT

Predictions of plasma parameters in the edge and scrape-off layer of tokamaks is difficult since most modern tokamaks have a divertor and the associated separatrix causes the usually employed field/fluxaligned coordinates to become singular on the separatrix/X-point. The presented field line map approach avoids such problems as it is based on a cylindrical grid: standard finite-difference methods can be used for the discretisation of perpendicular (w.r.t. magnetic field) operators, and the characteristic flute mode property  $(k_{\parallel} \ll k_{\perp})$  of structures is exploited computationally via a field line following discretisation of parallel operators which leads to grid sparsification in the toroidal direction. This paper is devoted to the discretisation of the parallel diffusion operator (the approach taken is very similar to the flux-coordinate independent (FCI) approach which has already been adopted to a hyperbolic problem (Ottaviani, 2011; Hariri, 2013)). Based on the support operator method, schemes are derived which maintain the selfadjointness property of the parallel diffusion operator on the discrete level. These methods have very low numerical perpendicular diffusion compared to a naive discretisation which is a critical issue since magnetically confined plasmas exhibit a very strong anisotropy. Two different versions of the discrete parallel diffusion operator are derived: the first is based on interpolation where the order of interpolation and therefore the numerical diffusion is adjustable; the second is based on integration and is advantageous in cases where the field line map is strongly distorted. The schemes are implemented in the new code GRILLIX, and extensive benchmarks and numerous examples are presented which show the validity of the approach in general and GRILLIX in particular.

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#### 1. Introduction

The modelling of the edge and scrape-off layer of tokamaks is in many ways more difficult than the core [1]. However, this region is of high importance since it may have a significant influence also on the core region, e.g. plasma and impurity densities are often largely set by edge conditions and in important operating conditions the edge plays a key role in the improvement of confinement [2]. Moreover, a prediction of heat fluxes on the divertor plates for future tokamaks is of high importance from the engineering point of view [3,4].

A major complexity at the modelling is introduced by the complex geometry of diverted machines. Field-aligned coordinates are often employed in simulations, since they allow for a convenient way to computationally exploit the characteristic flute mode property  $(k_{\parallel} \ll k_{\perp})$  of the structures. However, field-aligned coordinates become singular on the separatrix and simulations cannot

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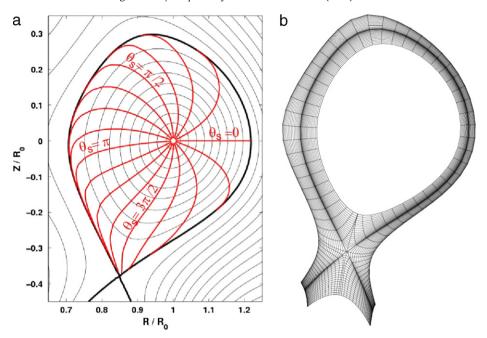
span a domain across it. Any set of poloidal  $(\theta_s)$  and toroidal  $(\varphi_s)$  straight field line angles has to satisfy along magnetic field lines the condition [5]:

$$\frac{d\theta_s}{d\phi} = \frac{1}{a(\phi)}. (1)$$

At the X-point the poloidal magnetic field vanishes and therefore on the separatrix the safety factor q diverges. The straight field line angles, which have to satisfy condition (1), cannot span the whole separatrix. As exemplified in Fig. 1(a) the contours of  $\theta_s$  are sucked into the X-point (see also [6]).

Also often employed are coordinates, where the field-alignment property is given up, but which is still aligned with flux surfaces, i.e.  $\rho(\psi)$  is retained as a radial coordinate. However, flux-aligned coordinate systems are still singular on points, where  $\nabla \psi = 0$ , i.e. at O-points and X-points [7]. Although these singularities can be cured numerically, O- and X-points remain somewhat exceptional points of the numerical grid (see Fig. 1(b)). This could in the worst case even lead to numerical artefacts. Moreover, structured flux-aligned meshes have a huge resolution imbalance within the

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**Fig. 1.** (a) Contours of flux label  $\rho$  (black) and poloidal straight field line angle  $\theta_s$  (red, symmetry coordinates) in diverted geometry for equilibrium from [16]. (b) Example for flux aligned mesh. The contours of the poloidal coordinate are orthogonal to flux surfaces. The X-point is connected to eight cells instead of the usual four cells. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

poloidal plane due to the flux expansion near the X-point [8,9]. Simulations might suffer from this as perpendicular operators arising in practically any plasma model (e.g.  $\nabla_{\perp}^2$ ,  $\mathbf{v}_E \cdot \nabla$ ) act approximately isotropically within poloidal planes of tokamaks.

The field line map approach is presented in Section 2. Although field/flux-aligned coordinates may become singular, the operators appearing in plasma models are still well defined, of course. The idea behind the approach is that the flute mode property can also be exploited at the discretisation step without any need for construction of a field/flux-aligned coordinate system. The approach consists of a cylindrical or Cartesian grid with a field line following discretisation for parallel operators. A separatrix can be treated as well as a magnetic axis, where X/O-points are treated like any other grid point and no resolution imbalance arises. The result is very similar to the flux-coordinate independent (FCI) [10–12] approach, and the derivation is here sketched without any reference to field- or flux-aligned coordinates.

As the discretisation of perpendicular operators in the field line map approach is straight forward, the main emphasis in this paper is on the discretisation of parallel operators. A hyperbolic problem has already been considered in [10,11], and this work is mainly devoted to the discretisation of the parallel diffusion operator in Section 2.4. Since an interpolation or integration is involved at the discretisation, parallel operators exhibit also numerical perpendicular 'diffusion'. Motivated by previous work from [13,14], a numerical scheme is developed which exhibits very low numerical diffusion. The discussion extends previous work from [15]. Several model problems are also discussed in the Appendix.

The developed numerical methods are implemented in the new code GRILLIX. In Section 3 extensive benchmarks performed with GRILLIX are presented, which show the validity of the field line map approach in general and GRILLIX in particular.

The paper is concluded with a summary and final remarks in Section 4.

#### 2. Field line map approach

#### 2.1. Overview

The field line map approach is described in the following for the case of a toroidal configuration  $(R, Z, \varphi)$ , but it can be applied

also to axial periodic configurations (x, y, z), where z is the axial coordinate. The transition should be trivial.

For a tokamak a cylindrical coordinate system is well defined everywhere, except for the toroidal symmetry axis which is outside the domain of interest. We span the simulation domain with a cylindrical grid  $R_i$ ,  $Z_j$ ,  $\varphi_k$ . (For axial configurations a Cartesian grid  $x_i$ ,  $y_j$ ,  $z_k$  is used.) Within each poloidal plane k the grid  $(R_i, Z_j)$  is Cartesian and bounded by extreme flux surfaces, which is the only dependence on flux surfaces of the approach. Based on the assumption of a strong toroidal field  $(B^{tor} \gg B^{pol})$ , any perpendicular operator is approximated by derivatives with respect to only R and R, but not R0. In order to exploit the flute mode property R1 R2, a dense resolution is chosen within poloidal planes, whereas the grid is sparsified along the R2 direction. The low resolution in R3 requires a field line following discretisation for parallel operators to achieve a sufficient directional accuracy for parallel operators.

It is noted that the assumption of a strong toroidal field is not a strictly necessary condition. If this assumption breaks down, a dense resolution also in  $\varphi$  would have to be retained, and the perpendicular operators would have to be adjusted to take into account also derivatives with respect to  $\varphi$ . Ultimately, the field line map approach would go over into a discretisation on a dense cylindrical grid, where the flute mode property would not be exploited any more. However, the method would still retain its validity.

#### 2.2. Perpendicular operators

Under the assumption of a strong toroidal field, any perpendicular operator can be approximated with derivatives with respect to only *R* and *Z*, e.g. the perpendicular Laplace operator becomes:

$$\nabla_{\perp}^{2} = \sum_{x^{n}, x^{m} = R, Z, \varphi} \frac{1}{R} \frac{\partial}{\partial x^{n}} \left[ R \left( g^{nm} - b^{n} b^{m} \right) \frac{\partial}{\partial x^{m}} \right]$$

$$\approx \frac{\partial^{2}}{\partial R^{2}} + \frac{\partial^{2}}{\partial Z^{2}} + \frac{1}{R} \frac{\partial}{\partial R}, \tag{2}$$

where  $g^{nm}$  the inverse metric of the cylindrical coordinate system and  $b^n$  the contravariant components of the unit vector of the

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