X-point modelling in linear configurations using BOUT++

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Abstract. Magnetic X-point configurations in tokamak geometries are critical in determining edge and scrape off layer (SOL) dynamics, and hence particle and heat flux onto plasma facing components. Alternative configurations have been proposed which aim to reduce fluxes to material surfaces, but their performance depends on cross-field transport in the region of the null point which is currently poorly understood. There is therefore a need for theoretical and experimental studies of turbulence in X-point magnetic configurations. In conventional 3D turbulence simulations of tokamaks, a field-aligned coordinate system is used, which introduces numerical instabilities at the null point due to zero volume elements. As a result, X-point dynamics are often interpolated based on nearby flux surfaces, which could exclude relevant physics. Here we simulate X-point configurations in linear geometries using a non-field-aligned coordinate system, and present results of 3D drift-wave turbulence and flow simulations in X-point configurations using an isothermal model which evolves density, vorticity, parallel velocity and parallel current density. Simulations have been performed to explore the feasibility of experimentally studying X-point configurations in linear plasma devices which indicate that even a modest coil set carrying 300A should produce a measurable effect on the driftwave turbulence and plasma profiles near the null region. The energy dynamics of the system are also explored and indicate that an X-point causes ohmic dissipation in higher mode number turbulence.

1. Introduction
There is growing concern that conventional divertor configurations in future devices could experience unacceptably high heat fluxes, especially during transient events [1, 2]. As a result, there have been studies into alternative concepts which could reduce the heat loads on divertor targets [3, 4]. The effectiveness of these configurations, however, are often sensitive to cross field transport in the null region, which is currently poorly understood [5].

Many of the current 3D plasma turbulence simulations do not directly model magnetic X-points, as they employ a field-aligned coordinate system [6, 7, 8]. The purely toroidal field at X-points creates numerical instability due to zero volume elements and therefore cannot be explicitly included in a field-aligned coordinate system. A common method is to interpolate plasma quantities from either side of the X-point region. This approach, however, could potentially exclude important physics associated with this region, such as mixing in the null region [9]. As a region of complicated plasma dynamics which can greatly affect the edge and SOL flows, the X-point region is an area which merits more detailed numerical study.
Alternatives to field-aligned coordinates, such as the Flux Coordinate Independent approach [10, 11] also ameliorates this issue, though its efficiency and accuracy are currently under investigation. While this is a functionality currently being implemented into BOUT++, this paper will address a simpler method of employing a cartesian coordinate system.

This paper is arranged as follows. The geometry and fluid model used in the following turbulence simulations are given in Section 2. Section 3 compares the turbulence characteristics and energy dynamics of a simple linear device to those of a device with X-point azimuthal fields, and Section 4 asserts our conclusions and future work.

2. Simulation geometry and model

2.1. Geometry and coordinate system

As an initial study into X-point simulation in BOUT++, we have considered a machine as shown in Figure 1. The machine parameters are chosen to correspond to a hypothetical university-scale experiment capable of producing X-points for tokamak-relevant scenarios. This machine will allow for direct investigation of fundamental plasma physics associated with tokamak divertor regions and allow simple diagnostic access to a null region, an area which is currently poorly understood. The machine parameters were chosen based on those achieved in previous machines [12, 13]. This device is proposed to produce low temperature, high density plasmas relevant to detachment and divertor-relevant scenarios. The electron temperature will be simulated as $T_{e0} \sim 2eV$, which is typical for linear devices as parallel streaming limits the maximum electron temperatures which can be achieved. The machine will achieve densities of up to $10^{19}m^{-3}$, as in previous machines [12, 14], for detachment-relevant scenarios. The initial plasma minor radius was considered to be 5cm. The axial magnetic field is $B_0 \sim 0.2 - 0.3T$.

An additional azimuthal field is created by longitudinal wires which can create X-point fields of approximately $B_{ext} \sim 0.02T$ at the edge of the simulation domain, which corresponds to a current of about 300A in the internal X-point wires, which are considered to be 18-turn coils. More exotic configurations such as the snowflake can easily be reproduced by the inclusion of more longitudinal wires. It should be noted that the interchange drive will not be present in this configuration, as there is no curvature. While this means that this machine will have different turbulent characteristics to a tokamak, it is still capable of producing tokamak-relevant studies applicable to divertor areas.

![Figure 1. Schematic of proposed device showing vessel and X-point coils. Cartesian coordinate system measuring 30cm x 30cm x 3m shown inlaid within the vessel. The four X-point coils are labelled with a ‘c’.](image)

In most 3 dimensional turbulence simulations, a field-aligned coordinate system is used in the interest of numerical efficiency. This method cannot be used to explicitly model X-points,
where the field is completely toroidal, as this introduces zero-volume elements. To ameliorate these issues, we have imposed a cartesian coordinate system, as shown in the centre of the machine pictured in Figure 1. The implementation of this coordinate system ensures that there are no zero volume elements, as each dimension is perpendicular to the other two, and therefore X-points (and any other singularities) can be effectively incorporated.

Figure 1 also illustrates the shape of the external field used to simulate X-point scenarios. This field was considered to be of the form shown in equation 1 [5], where $\theta = \tan^{-1}(\frac{z}{x})$ is the azimuthal angle. The magnitude and specific geometry of this field can be arbitrarily chosen by altering $A_0$, the exponent of r and corresponding coefficient of $\theta$.

$$A_{ext} = A_0 r^2 \cos(2\theta)$$

(1)

The expression in equation 1 then creates a perturbed field, as $B = \nabla \times A_{ext}$. The implementation of this perturbed magnetic field is described in section 2.3.

### 2.2. Isothermal Model

An isothermal cold-ion fluid model initially constructed for plasma blob studies [15, 16] is extended here to perform initial studies of X-point dynamics. The model is electrostatic, inviscid, and employs the Boussinesque approximation [17, 18]. It should also be noted that the results presented here are performed in a linear geometry ($\xi = \nabla \times \frac{b}{B} \rightarrow 0$), and therefore any terms involving curvature are neglected in the following analysis. Furthermore, the isothermal electron temperature $T_{e0}$ is 2eV. While this model includes several simplifications, it still captures relevant physics such as Kelvin-Helmholtz and driftwave turbulence, an important class of instabilities in tokamak edge plasmas [19], as it is a ubiquitous instability. The equations which are solved are given as follows in SI units:

- **Density continuity equation:**
  $$\frac{dN}{dt} = \nabla \cdot J - N_0 \nabla \cdot u$$  
  (2)

- **Vorticity:**
  $$\rho_s^2 N_0 \frac{d\Omega}{dt} = \nabla \cdot J + e$$
  (3)

- **Parallel velocity:**
  $$\frac{d u}{dt} = -c_s^2 \nabla \cdot n$$
  (4)

- **Ohm’s law:**
  $$J = \frac{\sigma T_{e0}}{e N_0} (\nabla \cdot N - N_0 \nabla \cdot \phi)$$
  (5)

Where $\Omega \equiv \nabla^2 \phi$ is vorticity, total derivatives are split via $\frac{d}{dt} = \frac{\partial}{\partial t} + u_E \cdot \nabla + u \cdot \nabla$, and parallel derivatives are evaluated using $\nabla \parallel = b \cdot \nabla$. In the above equations, $\rho_s = \frac{e \phi}{c_s}$ is the Bohm gyroradius. These equations are normalized such that density ($N$) is normalized to $N_0 = 5 \times 10^{18} m^{-3}$, speeds are normalized to the sound speed, and $\phi$ is the normalized electrostatic plasma potential. The boundary conditions for the simulations presented here will be discussed in section 3.

This model differs from that used in reference [16] in that it incorporates parallel ion free streaming, $u_\parallel$, as parallel flows are vital when determining the effects of X-points. Additionally, energy conservation required the restriction that $N$ is considered constant ($N_0$) in terms where it is not differentiated. See section 3.3 for a full discussion on the energy dynamics within the system.
2.3. Numerical Methods

This model was solved for the system described in section 2.1 using a resolution of 1.15mm \((1.25\rho_s)\) in the plane perpendicular to \(\mathbf{B} (x, z)\), and 8cm \((90.4\rho_s)\) in direction parallel to \(\mathbf{B} (y)\). The longitudinal direction was chosen to have a relatively low resolution, as fine structure dynamics were expected to be more dominant in the perpendicular planes. Previous studies of linear devices [20] have also indicated that low axial wave-numbers are dominant in linear configurations. Additionally, Alfvén lengthscales \((\frac{V_A}{\Omega_{ci}})\) are about 20cm, and therefore these dynamics are adequately resolved, as Alfvén wave transit times are shorter than perpendicular drift dynamics. The parallel dynamics introduced by the imposed X-point field were implemented by altering the \(\mathbf{b} \cdot \nabla\) operator such that \(\nabla_\parallel (f) \rightarrow \nabla_\parallel (f) - \left[ \frac{A_\parallel}{\mathbf{r} \cdot \mathbf{B}}, f \right]\), where the brackets indicate Poisson brackets, which were implemented using the Arakawa method [21]. Time integration was implemented using the implicit time integration solver CVODE, within the SUite of Nonlinear abd DIfferential/ALgebraic equation Solvers (SUNDIALS) [22]. Finally, the Laplacian solver, which calculates potential \((\phi)\) from vorticity \((\Omega)\), in BOUT++ was altered to invert using discrete sine transforms in the z direction (perpendicular to \(\mathbf{B}\) in the azimuthal plane), which eliminates the periodicity inherent in typical Laplacian inversion utilizing Fourier transforms.

3. Simulation analysis

3.1. Implementation and behavior

The model represented by equations 2 - 5 was implemented into BOUT++ and simulations were performed with and without an externally applied X-point field. The plasma source was modeled as a constant flow at the sound speed into the domain from one of the longitudinal boundaries \((y = 0)\). The opposing longitudinal boundary was considered to have zero-gradient boundary conditions in cases both with and without an imposed X-point. In cases with an X-point, sheath boundary conditions pertinent to presheath entrance as found in reference [23] were implemented. These boundary conditions are modified Bohm boundary conditions which account for the oblique magnetic fields at the Chodura sheath. As these boundary conditions rely on an oblique magnetic field, they could not be imposed in a basic linear case without an externally applied field. As such, these cases were constrained to zero-gradient boundary conditions on all fields in the directions perpendicular to the magnetic field.

Figure 2 shows the time evolution of the total energy of the fluctuations, which will be discussed later in Section 3.3. The simulations begin with an initial perturbation, and fluctuations grow until reaching a saturated, turbulent stage. This stage is shown in as the flat section in Figure 2. All analysis presented in this work has been conducted within this regime.

Figure 3 illustrates the mean radial density profiles both with (solid) and without (dotted) an X-point at various locations along the length of the device. The radial profiles in each case is taken along a diagonal \((x = z)\) line across the azimuthal plane which lies on the X-point. Figure 3 indicates that the introduction of a magnetic X-point introduces an asymmetric off-axis peak of density and a narrowing of the total profile.

The narrowing of the profiles induced by the X-point as shown in Figure 3 can be attributed to the externally applied azimuthal magnetic field, which is shown in Figure 4. The profile is distorted due to the external magnetic field which maps a circular input profile to an elongated profile at the opposite (sheath) end. This can be described by simply following field lines. As one moves along the axis of the machine, the perturbed field shifts the total magnetic field such that it is closer to the null point in two directions (top right and bottom left in Figure 4). This therefore creates a narrowing of the profiles in that direction. Likewise the opposite occurs in the other two directions, creating a broadened radial density distribution. Finally, Figure 3 also indicates that the radial density profiles are smoother without an X-point field applied. This
3.2. Transport and cross correlation

To study the parallel dynamics of the system, cross correlation analysis was employed. The inbuilt cross correlation function in IDL was used to compute the cross correlation \( P_{fg} \) of two quantities \( f \) and \( g \) using the method shown in equation 6. Here \( k \) is the index for each population and \( M \) is the number of elements in said population.

\[
P_{fg} = \sum_{k=0}^{M-1} (f_k - \bar{f})(g_k - \bar{g}) \left\{ \left[ \sum_{k=0}^{M-1} (f_k - \bar{f})^2 \right] \left[ \sum_{k=0}^{M-1} (g_k - \bar{g})^2 \right] \right\}^{-\frac{1}{2}} \tag{6}
\]

Using this method, one can determine the correlation between two quantities at different points within the domain. This serves as a convenient method to visualize flow dynamics, as

could perhaps be explained by considering the cross field transport introduced by the X-point which inhibits the azimuthal flow of plasma, forcing coherent structures to dissolve.
shown in Figure 5, which shows the two dimensional density cross correlations in an azimuthal plane at the center of the machine \((y = 1.5m)\) when an X-point field is applied. This figure illustrates the effects of an induced X-point on parallel dynamics, as flows are apparent along field lines. The reference point in Figure 5 is shown in black near the null region.

Figure 6 plots the cross field flux \((\Gamma)\) when an X-point is applied, given by \(\Gamma = \langle N v_\perp \rangle\) where \(v_\perp = \frac{\|b \times \nabla \tilde{\phi}\|}{B}\) and \(\tilde{\phi} = \phi - \langle \phi \rangle\). The cross field flux indicates the regions of high cross field transport, which is an important factor in the effectiveness of novel divertor configurations such as the snowflake [5].

**Figure 5.** Two dimensional cross correlation at \(y=1.5m\), reference point shown as black dot.

**Figure 6.** Cross field flux at \(y=1.5m\), indicating that the center of the machine is the dominant area for cross-field transport.

Figures 5 and 6 indicate two characteristics of note. Firstly, Figure 5 indicates that away from the null point, flows remain along field lines, being highly correlated to positions parallel to field lines, but adjacent areas perpendicular to field lines are less correlated. Secondly, Figure 6 indicates that the null point is the main area of cross-field transport allowing plasma to flow from one region to another.

Furthermore, the effect of the imposed X-point on the system’s turbulence can be examined using basic synthetic diagnostics. Specifically, one can look at the turbulence at a constant radius from the center of the plasma column, in this case considered to be \(r = 5cm\), and measure the phase shift between potential and density fluctuations. Figures 7 and 8 indicate this relationship measured on turbulence with longitudinal fluctuations (driftwave-like), which was chosen due to its ubiquitous nature. [19, 24]

It is clear in Figures 7 and 8 that the induced X-point introduces a broadening in the turbulent spectrum. This is to be expected, as the perpendicular, perturbed X-point field lines inhibit the transport of turbulent structures, and therefore decorrelate adjacent fluctuations.

### 3.3. Energy dynamics

An analysis of the energy dynamics within the system was performed similar to that found in reference [25]. In this work, the system is spectrally-decomposed in the azimuthal and axial directions, and the energy of each mode is analyzed to determine the energy transfer channels and dissipation. The energy of each Fourier mode where \(\vec{k} = (m, n)\), with \(m\) being the poloidal mode number and \(n\) the axial mode number, is:
Figure 7. Phase shift comparison of density and potential perturbations in driftwave-like modes in a basic linear geometry.

Figure 8. Phase shift comparison of density and potential perturbations in driftwave-like modes with an applied X-point.

Figure 9. Phase shift profiles averaged over $\rho_k$.

\[ E_{\text{tot}}(k) = \frac{1}{2} \left( |N_k|^2 + \frac{1}{2} |u_{||,k}|^2 + \rho_s^2 \frac{1}{2} \left( \left| \frac{\partial \phi_k}{\partial r} \right|^2 + \frac{m^2}{r^2} \left| \phi_k \right|^2 \right) \right) \] (7)

Where $N_k$, $u_{||,k}$ and $\phi_k$ are the Fourier-transposed density, parallel velocity, and potential, respectively. The analysis presented here occurs in the turbulent, steady state phase described in Figure 2. The individual terms in equation 7 indicate the (a) internal energy, (b) parallel kinetic energy, and (c) perpendicular kinetic energy of the system in Fourier space. The evolution of each Fourier mode can be described as [25]:

\[ \frac{\partial E_f(k)}{\partial t} = Q_f(k) + C_f(k) + D_f(k) \] (8)

Here, $f$ indicates each field ($N, u_{||}, \phi, j_{||}$), and $Q_f(k)$, $C_f(k)$, and $D_f(k)$ stand for the nonconservative energy forces (i.e. external sources and sinks), linear energy transfer channels, and dissipation terms respectively. There are only conservative energy forces in our system, so $Q_f(k) = 0$. The exact expressions for $C_f(k)$ and $D_f(k)$ are:
\[ C_N(\vec{k}) = \frac{1}{eN_0^2} \text{Re} \left\langle ik\|j\|,\vec{k}N_k^2 \right \rangle \]  
(9)

\[ C_\phi(\vec{k}) = \frac{1}{eN_0^2} \text{Re} \left\langle ik\|j\|,\vec{k}\phi_k^* \right \rangle \]  
(10)

\[ C_u(\vec{k}) = \frac{1}{N_0} \text{Re} \left\langle ik\|N_k^2,\vec{k}u_k^* \right \rangle \]  
(11)

\[ C_j(\vec{k}) = \frac{1}{eN_0^2} \text{Re} \left\langle ik\|N_k^3j_k^* - iN_0k\|\phi_k^*j_k^* \right \rangle \]  
(12)

\[ D_j(\vec{k}) = \text{Re} \left\langle \frac{-j_k^2}{\sigma T_e} \right \rangle \]  
(13)

Figure 10. Energy dynamics diagram indicating the transfer of energy via sound waves and adiabatic drift waves.

Furthermore, our system conserves energy except for ohmic dissipation, \( \sum_f C_f(\vec{k}) = 0 \), as shown in Figure 10. As a result, equation 8 elucidates the wavenumbers at which energy is dissipated from the system, as the only terms remaining are those found in \( D_f(\vec{k}) \). Figures 11 and 12 plot the nonconservative rate of change of the total energy, \( \frac{\partial E_f(\vec{k})}{\partial t} \), as a function of wavenumber in cases with and without an X-point.

These results are similar to those found in [25] in that the energy dynamics (in this case dissipation) is localized to small longitudinal mode numbers. It should be noted that the nonconservative rate of change of our total energy is negative, as the only contribution is from the ohmic dissipation, \( D_j \). Furthermore, and somewhat unexpectedly, an X-point reduces the dissipation in higher n-numbers, indicating that the azimuthally-applied X-point perturbs the strictly parallel mode number dissipation. This could perhaps be explained by considering the distortion of the profiles as shown in Figure 4.

Figures 13 and 14 show the nonconservative rate of change of the total energy at selected longitudinal mode numbers as a function of azimuthal mode number. It is clear from these plots that the n=0 mode is dominant across the azimuthal mode number spectrum both with and without an X-point. While the introduction of an X-point induces a shift of dissipation to lower n-numbers, Figures 13 and 14 indicate that dissipation increases for each of those lower-n modes.
4. Conclusions and future work

BOUT++ can capably handle direct X-point simulations by imposing a simple cartesian coordinate system and altering parallel operators to include perturbed external fields. The introduction of a modest magnetic X-point perturbs the turbulence characteristics of the plasma column and alters the energy dynamics within the system. The simulations presented here indicate that a simple langmuir probe in such a device would be able to distinguish an altered driftwave phase shift, and measure a perturbed density profile exhibiting transport along the X-point field lines.

The Flux Coordinate Independent (FCI) method currently being implemented into BOUT++ could potentially offer a more efficient method to capably handle magnetic X-point regions. In addition, the implementation of a more complex model which includes temperature evolution will allow studies of heat and energy convection which could elucidate physics relevant to novel divertor configurations. With this model and the implementation of the FCI method, full tokamak simulations including explicit magnetic X-point simulation could be accomplished using BOUT++.
References

[1] G Federici, A Loarte, and G Strohmayer. Assessment of erosion of the iter divertor targets during type i elms. *Plasma physics and controlled fusion*, 45(9):1523, 2003.

[2] A Zhitlukhin, N Klimov, I Landman, J Linke, A Loarte, M Merola, V Podkovyrov, G Federici, B Bazylev, S Pestchanyi, et al. Effects of elms on iter divertor armour materials. *Journal of nuclear materials*, 363:301–307, 2007.

[3] S I Krasheninnikov, A Y Pigarov, and D J Sigmar. Plasma recombination and divertor detachment. *Physics Letters A*, 214(5):285–291, 1996.

[4] P M Valanju, M Kotschenreuther, S M Mahajan, and J Canik. Super-x divertors and high power density fusion devices. *Physics of Plasmas*, 16(5):056110–056110, 2009.

[5] D D Ryutov, R H Cohen, T D Rogaljen, and M V Umansky. A snowflake divertor: a possible solution to the power exhaust problem for tokamaks. *Plasma Physics and Controlled Fusion*, 54(12):124050, 2012.

[6] B D Dudson, M V Umansky, X Q Xu, P B Snyder, and H R Wilson. BOUT++: A framework for parallel plasma fluid simulations. *Computer Physics Communications*, 180:1467–1480, 2009.

[7] P Ricci, F D Halpern, J Loizu, A Mosetto, A Fasoli, I Furno, and C Theiler. Simulation of plasma turbulence in scrape-off layer conditions: the gbs code, simulation results and code validation. *Plasma Physics and Controlled Fusion*, 54(12):124047, 2012.

[8] B D Scott. Free-energy conservation in local gyrofluid models. *Physics of Plasmas (1994-present)*, 12(10):–, 2005.

[9] W A Farmer and D D Ryutov. Axisymmetric curvature-driven instability in a model divertor geometry. *Physics of Plasmas (1994-present)*, 20(9):–, 2013.

[10] F Hariri and M Ottaviani. A flux-coordinate independent field-aligned approach to plasma turbulence simulations. *Computer Physics Communications*, 184(11):2419 – 2429, 2013.

[11] F Hariri, P Hill, M Ottaviani, and Y Sarazin. The flux-coordinate independent approach applied to x-point geometries. *Physics of Plasmas (1994-present)*, 21(8):–, 2014.

[12] B Mihalji, P K Browning, and K J Gibson. Spatially resolved spectroscopy of detached recombining plasmas in the university of manchester linear system divertor simulator. *Physics of Plasmas (1994-present)*, 14(1):–, 2007.

[13] J C Sandeman, P Uddholm, J A Elliott, and M G Rusbridge. Experiments on drift wave launching: I. dispersion curves and damping rates. *Physics of Plasmas and Controlled Fusion*, 39(1):159, 1997.

[14] W Gekelman, H Pfister, Z Lucky, D Bamber, Jand Leneman, and J Maggs. Design, construction, and properties of the large plasma research devicethe lapd at ucla. *Review of Scientific Instruments*, 62(12):2875–2883, 1991.

[15] J R Angus, M V Umansky, and S I Krasheninnikov. Effect of drift waves on plasma blob dynamics. *Physical Review Letters*, 108(21):215002, 2012.

[16] N R Walkden, B D Dudson, and G Fishpool. Characterization of 3d filament dynamics in a mast sol flux tube geometry. *Plasma Physics and Controlled Fusion*, 55(10):105005, 2013.

[17] J R Angus and M V Umansky. Modeling of large amplitude plasma blobs in three-dimensions. *Physics of Plasmas (1994-present)*, 21(1):–, 2014.

[18] G Q Yu, S I Krasheninnikov, and P N Guzdar. Two-dimensional modelling of blob dynamics in tokamak edge plasmas. *Physics of Plasmas (1994-present)*, 13(4):–, 2006.

[19] B D Scott. The nonlinear drift wave instability and its role in tokamak edge turbulence. *New Journal of Physics*, 4(1):52, 2002.

[20] M. V. Umansky, P. Popovich, T. A. Carter, B. Friedman, and W. M. Nevins. Numerical simulation and analysis of plasma turbulence the large plasma devicea). *Physics of Plasmas (1994-present)*, 18(5):–, 2011.

[21] A Arakawa and V R Lamb. Computational design of the basic dynamical processes of the [UCLA] general circulation model. In J Chang, editor, *General Circulation Models of the Atmosphere*, volume 17 of *Methods in Computational Physics: Advances in Research and Applications*, pages 173 – 265. Elsevier, 1977.

[22] Advanced computational software collection, us doe.

[23] J Loizu, P Ricci, F D Halpern, and S Jolliet. Boundary conditions for plasma fluid models at the magnetic presheath entrance. *Physics of Plasmas (1994-present)*, 19(12):–, 2012.

[24] B Friedman, T A Carter, M V Umansky, D Schaffner, and B Dudson. Energy dynamics in a simulation of lapd turbulence. *Physics of Plasmas (1994-present)*, 19(10):–, 2012.