Name of Bidding Organisation:	University of Oxford
Contract Title:	FM-WP2 Plasma Multiphysics model: Development of gyro-averaged referent model (Project NEPTUNE)

1 Purpose of Document

This document provides a statement of how and when the Research Plan's objectives would be achieved, by showing the major products, activities and resources required of the Research Plan.

2 Benefits and alignment to Work Package objectives

Please evidence below how the submission aligns to the Work Package objectives outlined in Part 1 Section 1.3.

- We will develop different drift kinetic models applicable to the plasma edge and compare them in various simplified settings to propose a referent model, which is one of the stated purposes of Work Package FM-WP2.
- The different drift kinetic approaches will be tested in proxy-apps that will solve the drift-kinetic equivalent of the following problems (numbering corresponds to the one used in the document Fusion Modelling System Science Plan):

  4. Spatially 1D plasma model incorporating velocity space effects.

  6. Spatially 2D plasma model incorporating velocity space effects.

  These problems are of interest for Work Package FM-WP2.
- We will include a simplified model for neutrals to see how it affects the plasma behaviour. This will facilitate future interaction with FM-WP3.
- As asked in section 1.3 of part 1, we will consider geometries (i)-(iv) (slab-twisted/toroidal) by ultimately constructing a model for helical magnetic fields.
- As asked in section 1.3 of part 1 of the bid, we will construct our models so that they transition smoothly from core δf gyrokinetics to drift kinetics and from drift kinetics to fluid equations as the "magnetisation" parameter δ_s and normalised collision frequency ν^* change across the edge plasma.
- As asked in section 1.3 of part 1 of the bid, we will develop boundary conditions to connect to the non-neutral sheaths that cover the walls of the tokamak, and we will discuss how to connect to fluid equations and δf gyrokinetics.

3 Scope

3.1 Key Deliverables and/or Desired Outcomes

- Report describing the important regimes in the tokamak plasma edge and a review of the state-of-the-art, including prioritisation of key physical processes for modelling and for further research, as requested in section 2.1 of part 1 of the bid.
- Proxy-app that compares different drift kinetic models for a spatially 1D plasma.
- Proxy-app that compares different drift kinetic models for a spatially 2D plasma.
- Report on the full drift kinetic model for helical magnetic field, including material to assist numerical implementation and a discussion of possible extensions of the model.

3.2 Exclusions

Activities/topic areas that are out of scope of the Bid and which will not be undertaken (may also include things that Bidder would like to do but are not currently in scope)

- We will develop a model for helical magnetic fields to ensure that we include toroidicity into the problem, but we do not propose to develop a model for a full tokamak magnetic field. We have two reasons to justify this strategy:

  (i) helical magnetic fields are the current state-of-the-art for edge kinetic codes [N. R. Mandell et al, *J. Plasma Phys.* **86**, 905860109 (2020)], and

  (ii) very recent work suggests that the radial components of the curvature and ∇B drifts have been treated improperly in previous edge plasma models [J. F. Parisi et al, accepted in *Nucl. Fusion*, https://arxiv.org/abs/2004.13634].

  More research, outside of the scope of this bid, is needed to determine the correct way to introduce the radial components of the curvature and ∇B drifts into drift kinetic models for the edge.

3.3 Constraints

Restrictions that affect proposals of the project by imposing limitations such costs, resources or project schedule, which may affect the execution of the Bid.

- The proposed time commitment of Professors Felix I. Parra Diaz and Michael Barnes has been calculated to ensure that they are able to be relieved of some of their teaching duties for the duration of the project. Any reduction in the funds might lead to a very sharp reduction in the deliverables.

4 Approach

Describe how will the work be undertaken, including a definition of methodology that will be used in the project to deliver the work package and call objectives.

We propose the development of an electrostatic drift-kinetic model for a magnetized plasma in a helical magnetic field composed of one ion species, electrons and one neutral species. Drift kinetics is an expansion in the "magnetisation" parameter δ_s that eliminates the fast gyro-orbit timescale and one of the velocity space coordinates: the gyrophase [1]. Our proposal addresses four challenges that are crucial for drift kinetic treatments of the edge plasma:

- Unfortunately, a piece of the electric field (the radial component) cannot be determined with the lowest order drift kinetic equations [2]. Higher order terms have to be kept, and the most common way to do so is to split the distribution function and the electromagnetic fields into a background, slowly varying piece and a fast-evolving, small piece: δf gyrokinetics [3, 4]. This procedure is not valid for edge plasmas. As a result, terms of different order in the expansion must be included in the model for edge plasmas, leading to equations with terms of very different size and hence to numerical constraints. For example, the time step size in electrostatic drift kinetics is heavily constrained by an uninteresting and unphysical wave known as the electrostatic shear Alfven wave [5, 6].
- Drift kinetic formulations are valid everywhere in the edge, but they are overly complicated for the core, where δf gyrokinetics should be applied, and for the far scrape-off layer, where collisions are frequent and fluid models can be used [7]. It would be highly desirable to have an edge drift kinetic

model that smoothly converts into these other simpler, faster models for the tokamak core and the far scrape-off layer.

- To our knowledge, the drift kinetic expansion in the presence of a wall has only been considered recently [8], and it needs to be developed further.
- To our knowledge, drift kinetic expansions have not been performed including neutral physics. The inclusion of neutrals breaks the usual drift kinetic expansion because neutrals are not magnetised and hence can introduce dependence on the gyrophase back into the equations.

To address the first two points, we propose a new method to derive drift kinetics. Instead of working with the distribution function $f(\mathbf{x}, \mathbf{v}, t)$ that depends on position $\mathbf{x}$, velocity $\mathbf{v}$ and time t, we will develop a gyrokinetic set of equations that will evolve the normalized distribution function $F(\mathbf{x}, \mathbf{w}, t) = (v_{th}^3/n) f(\mathbf{x}, \mathbf{w}v_{th} + \mathbf{u}, t)$ that depends on the normalized velocity $\mathbf{w} = (\mathbf{v} - \mathbf{u})/v_{th}$. Here n is the particle density, $\mathbf{u}$ is the average velocity and v_{th} is the thermal speed. The values of n, $\mathbf{u}$ and v_{th} will be obtained from fluid-like equations. We expect this approach to have three advantages:

- The higher order terms required to obtain the radial component of the electric field will only appear in one of the equations. This equation can be numerically evolved with implicit time-stepping methods to avoid numerical problems that stem from terms of very different size co-existing in the same equation.
- Using the fluid equations for n, $\mathbf{u}$ and v_{th}, it is easier to impose conservation of global energy and momentum. Unlike other moment approaches based on polynomial expansions of f, our proposed approach will ensure that f remains positive.
- The fact that n, $\mathbf{u}$ and v_{th} are evolved independently makes matching with fluid equations and with δf gyrokinetics straightforward.

There are risks associated with the development of a new approach to drift kinetics. To mitigate those risks, in the initial stages of the project, we will compare the new approach with more conventional drift kinetic equations by implementing both approaches in one proxy-app. In this way, we can easily revert to conventional drift kinetics if necessary. We propose to build four proxy-apps to test the most important features of the new set of equations:

1. **1D model along straight magnetic field lines with periodic boundary conditions.** The idea is to start with a simple proxy-app to test the new drift kinetic approach. The usual 1D drift kinetic equation will be compared with three other models:
    a. One in which the density n is evolved using a fluid-like equation.
    b. One in which both the density n and the average velocity $\mathbf{u}$ are evolved using fluid-like equations.
    c. One in which the density n, the average velocity $\mathbf{u}$ and the thermal speed v_{th} are evolved using fluid-like equations.

    With this approach, we will test whether our proposed method to obtain drift kinetic equations leads to unforeseen numerical problems. We will also test different implicit time evolution algorithms by treating implicitly only some terms in the fluid-like equations for n, $\mathbf{u}$ and v_{th}. If we find numerical problems that are insurmountable, we will revert to the usual derivation of drift kinetics.

    The piece of the electric field that necessitates the inclusion of higher order terms in the drift kinetic equation is perpendicular to the magnetic field. Thus, in this 1D proxy-app we will not need to include terms of very different sizes.

    The proxy-app will be benchmarked against analytical solutions for Landau damping of ion acoustic waves.

2. **1D model along straight magnetic field lines with wall boundary conditions.** We want to develop a drift kinetic model in the presence of walls. This means imposing boundary conditions at the end of magnetic field lines that represent such walls [8]. This proxy-app will test the compatibility between the wall boundary conditions and the new drift kinetic approach with fluid-like equations for density, average velocity and thermal speed.

   The piece of the electric field that necessitates the inclusion of higher order terms in the drift kinetic equation is perpendicular to the magnetic field. Thus, in this 1D proxy-app we will not need to include terms of very different sizes.

   The proxy-app will be benchmarked against analytical steady state solutions obtained for particular particle sources [9, 10], and against analytical time-evolving solutions obtained for particular initial conditions [11, 12].

3. **Axisymmetric 2D model with helical field lines and wall boundary conditions.** This 2D model does not include turbulence due to axisymmetry and hence all the transport will be collisional in nature. To avoid having to include finite orbit width effects, we will assume that collisions with neutrals produce most of the transport. This limit is relevant to tokamaks, as it corresponds to the charge exchange mean free path being larger than the ion gyroradius.

   This 2D model will allow us to test the compatibility of the new drift kinetic approach with 2D geometry. The wall boundary conditions determine the piece of the electric field that necessitates the inclusion of higher order terms in the drift kinetic equation. Thus, in this proxy-app we will not need to include terms of very different sizes.

   We have decided to limit our proxy-app to helical magnetic field lines because this is the current state-of-the-art for edge kinetic codes [13] and because in this way we avoid having to choose an ordering for the radial components of the curvature and ∇B drifts. These drifts have been neglected in the past, but recently their radial components have been proven to be important in JET pedestals [14]. Further research is needed to determine the importance of these radial components, and this is outside of the scope of this proposal.

   We will benchmark this 2D model with analytical solutions in the high collisionality regime (fluid limit) [7].

4. **Axisymmetric 2D model with helical field lines and periodic boundary conditions.** The periodic boundary conditions imitate the closed flux surfaces in the tokamak core. Due to the periodic boundary conditions, there is a perpendicular component of the electric field (the radial component) for which we need higher order terms. We will test whether our new approach to drift kinetics facilitates the calculation of this component.

   We will benchmark this 2D model with analytical solutions in the high collisionality regime (fluid limit) [7].

During each stage, we will re-evaluate the numerical approach taken to ensure that it is efficient. We will endeavour to design each proxy-app to be as modular as possible to enable testing of different models/numerical approaches and to improve portability.

In addition to the two axisymmetric 2D proxy-apps with different boundary conditions, we will consider an axisymmetric plasma with two spatial regions: one with periodic boundary conditions (tokamak core) and another with wall boundary conditions (Scrape-Off Layer). We will determine the appropriate equations for the transition between these two regions. Note that the radial electric field is determined differently on each side of the 'separatrix' between the two regions.

The interactions between the neutrals and the charged particles will be modelled using Krook operators. By using simplified models for collisional interactions between charged particles and neutrals, we are able to focus on the drift kinetic treatment, while still keeping important neutral effects.

The final result of our process will be a 3D electrostatic referent drift kinetic model for helical magnetic fields. Note that we will have only built 2D proxy-apps, but the model will be fully 3D. We believe that we have chosen proxy-apps that will uncover most of the numerical problems that can be associated with the new drift kinetic approach. If the new approach to drift kinetics does not work due to unforeseen numerical problems, we will derive a new drift kinetic model with all the higher order terms needed to calculate every component of the electric field.

In addition to providing an electrostatic referent model for helical magnetic fields, we will write a report discussing three possible extensions: the inclusion of gyroaverages to convert the drift kinetic model into a gyrokinetic model, the inclusion of radial magnetic drifts, and the inclusion of electromagnetic effects.

References

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[2] F. I. Parra and P. J. Catto, *Plasma Phys. Control. Fusion* **50**, 065014 (2008).
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[7] P. Helander, S. I. Krasheninnikov and P. J. Catto, *Phys. Plasmas* **1**, 3174 (1994).
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[11] J. E. Allen and J. G. Andrews, *J. Plasma Phys.* **4**, 187 (1970).
[12] N. St. J. Braithwaite and L. M. Wickens, *J. Plasma Phys.* **30**, 133 (1983).
[13] N. R. Mandell et al, *J. Plasma Phys.* **86**, 905860109 (2020).
[14] J. F. Parisi et al, accepted in *Nucl. Fusion*, https://arxiv.org/abs/2004.13634.

5 External Dependencies

Information about potential dependencies on other activities/organisations involved eg. Data that would need to have access to as part of the research, what historical data would be available to run case studies, that the Bid would benefit from

Dependency Description	**Responsible Owner**	**Required Data**

6 Activity Plan

Identify activities plans for the Research Plan (please add and use as many activity templates as required into the document and complete Annex B with schedule). Please include any relevant planning assumptions.

Duplicate this table for each Activity	**Activity No**	**1**
<u>Activity:</u>		

Development of drift kinetic referent model **Assignee:** Felix I. Parra Diaz		
Objective 1: Identify the theoretical work that needs to be done to obtain a complete drift kinetic referent model for the edge. **Objective 2:** Propose a drift kinetic referent model for helical magnetic field lines. **Objective 3:** Propose a suite of theoretical tests for the drift kinetic referent model.		
Key Deliverables:	**Start and Completion date:**	**Assignee:**
1) Report describing the important regimes in the tokamak plasma edge and a review of the state-of-the-art, including prioritisation of key physical processes for modelling and for further research.	**1)** Jan. 2021 – March 2021	**1)** Felix I. Parra Diaz
2) Report on 1D model along magnetic field lines with periodic boundary conditions and with wall boundary conditions	**2)** Jan. 2021 – May 2021	**2)** Felix I. Parra Diaz
3) Report on axisymmetric 2D model with wall boundary conditions	**3)** March 2021 – Sept. 2021	**3)** Felix I. Parra Diaz
4) Report on axisymmetric 2D model with periodic boundary conditions	**4)** Aug. 2021 – Nov. 2021	**4)** Felix. I. Parra Diaz
5) Report on axisymmetric 2D model with 'separatrix'	**5)** Nov. 2021 – Jan. 2022	**5)** Felix I. Parra Diaz
6) Report on the 3D electrostatic referent model for a helical magnetic field	**6)** Jan. 2022 – May 2022	**6)** Felix I. Parra Diaz
7) Report on extensions to the 3D electrostatic referent model for helical magnetic field	**7)** March 2022 – June 2022	**7)** Felix I. Parra Diaz
Milestones towards deliverables:	**Completion date:**	**Assignee:**
1) Report on 1D model along magnetic field lines with periodic boundary conditions	**1)** Jan. 2021	**1)** Felix I. Parra Diaz
2) Report describing the important regimes in the tokamak plasma edge and a review of the state-of-the-art, including prioritisation of key physical processes for modelling and for further research.	**2)** March 2021	**2)** Felix I. Parra Diaz
3) Report on wall boundary conditions	**3)** May 2021	**3)** Felix I. Parra Diaz

4) Report on 2D model with wall boundary conditions **5)** Report on fluid analytical solutions to use as benchmarks for the 2D model with wall boundary conditions **6)** Report on 2D model with periodic boundary conditions **7)** Report on 2D model with 'separatrix' **8)** Report on the 3D electrostatic referent model for helical magnetic field **9)** Modifications to the 3D electrostatic referent model for helical magnetic field suggested by proxy-app results **10)** Report on extensions to the 3D electrostatic referent model for helical magnetic field	**4)** July 2021 **5)** Sept. 2021 **6)** Nov. 2021 **7)** Jan. 2022 **8)** March 2022 **9)** May 2022 **10)** June 2022	**4)** Felix I. Parra Diaz **5)** Felix I. Parra Diaz **6)** Felix I. Parra Diaz **7)** Felix I. Parra Diaz **8)** Felix I. Parra Diaz **9)** Felix I. Parra Diaz **10)** Felix I. Parra Diaz

Duplicate this table for each Activity	**Activity No**	2
<u>Activity:</u> Implementation and testing of the drift kinetic referent model **<u>Assignee:</u>** Michael Barnes		
<u>Objective 1:</u> Compare the numerical performance of the novel, moment-based drift kinetic model to a more standard drift kinetic model for a variety of problems. **<u>Objective 2:</u>** Determine potential bottlenecks in the numerical treatment of the drift kinetic models **<u>Objective 3:</u>** Develop appropriate numerical algorithms for treating the wall boundary		
<u>Key Deliverables:</u> **1)** Proxy-app for 1D drift kinetic model **2)** Report on numerical issues and findings associated with the 1D drift kinetic models **3)** Proxy-app for 2D drift kinetic model **4)** Report on numerical issues and findings associated with the 2D drift kinetic model	**<u>Start and Completion date:</u>** **1)** Jan. 2021 **–** Sept. 2021 **2)** Jan. 2021 **–** Oct. 2021 **3)** Oct. 2021 **–** June 2022 **4)** Oct. 2021 **–** June 2022	**<u>Assignee:</u>** **1)** Michael Barnes **2)** Michael Barnes **3)** Michael Barnes **4)** Michael Barnes

5) Final report on the developed Proxy-apps	**5)** Oct. 2021 **–** June 2022	**5)** Michael Barnes
<u>Milestones towards deliverables:</u> **1)** Report on numerical issues/findings for standard 1D drift kinetic code with periodic boundary conditions **2)** Report on numerical issues/findings for simplest (only density) moment-based 1D model with periodic boundary conditions **3)** Report on numerical comparison between standard and moment-based 1D models **4)** Report on numerical issues/findings for standard 1D drift kinetic code with wall boundary conditions **5)** Report on numerical issues/findings for moment-based 1D model with wall boundary conditions **6)** Report on numerical issues/findings for standard 2D model with wall boundary conditions **7)** Report on numerical issues/findings for moment-based 2D model with wall boundary conditions **8)** Report on numerical issues/findings for 2D model with periodic boundary conditions **9)** Final report on numerical issues/findings from the developed Proxy-apps	**<u>Completion date:</u>** **1)** Feb. 2021 **2)** April 2021 **3)** June 2021 **4)** Aug. 2021 **5)** Oct. 2021 **6)** Dec. 2021 **7)** Feb. 2022 **8)** April 2022 **9)** June 2022	**<u>Assignee:</u>** **1)** Michael Barnes **2)** Michael Barnes **3)** Michael Barnes **4)** Michael Barnes **5)** Michael Barnes **6)** Michael Barnes **7)** Michael Barnes **8)** Michael Barnes **9)** Michael Barnes