Overview of the numerical issues and findings associated with the 1D and 2D drift kinetic models

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1. Introduction

An accurate model of plasma dynamics in the edge of tokamaks must include a treatment of both open and closed field lines, motion both along and across the (predominantly toroidal) equilibrium magnetic field, and interaction between charged and neutral particles. As the plasma varies from nearly collisionless in the closed-field-line region to strongly collisional close to the material wall, the model should further incorporate kinetic effects and – ideally – reduce to a fluid description where appropriate. We considered a variety of different drift kinetic models for this project, each addressing different aspects of the physics needed to probe key features of plasma dynamics in the edge of tokamaks. The results of our numerical studies of these models is contained in a series of reports [1, 2, 3, 4, 5, 6, 7, 8], culminating in overviews of both drift kinetic and moment kinetic models for parallel dynamics [7] and a drift kinetic model for dynamics in a homogeneous, helical magnetic field [8]. In particular, for details on the current state of our most physically-complete numerical model, see [8]. Rather than re-hashing the details of those reports here, we instead provide what we think are key findings from our numerical studies, including a discussion of numerical difficulties encountered, how they were (or were not) overcome, outstanding issues and possible next steps.

2. Space-time discretisation

For all model varieties we considered, we chose to discretise in time using a time-marching scheme taken from the family of Strong Stability Preserving Runge-Kutta schemes and in space using Chebyshev spectral elements. We chose these discretisations for a combination of robustness, ease of implementation and computational efficiency. This discretisation worked well in most of the cases we considered, with good convergence properties; c.f. [7]. However, we did sometimes find it necessary to use upwinded fluxes at element boundaries in order to ensure numerical stability. We also observed poor convergence near the domain boundary for cases with a helical field and non-zero radial electric field; this is discussed separately below.

Other than a simple finite-difference discretisation in space, which performed predictably poorly relative to the spectral element approach in virtually all cases, no other methods were attempted. Though beyond the scope of our study, it may thus prove profitable to explore other discretisations.

It is perhaps worth noting that as part of our algorithm, we developed a scheme for ensuring exact conservation of particles, momentum and energy (where appropriate), c.f. [7]. This scheme generically improved numerical stability and was particularly necessary to maintain stability for the moment kinetic model. At present, the method of guaranteeing conservation properties involves correcting the nominal distribution function with a function whose form is constrained to be similar to a Maxwellian distribution in velocity space. Given that the actual distribution function may be far from Maxwellian in regions of the edge plasma, it may be worth generalising the form of the correction used in the code.

3. Moment kinetic approach

One of the main aims of our numerical investigation was to evaluate the efficacy of a novel moment kinetic model for simulating edge plasma dynamics. This model has the advantage of decoupling the density, flow and pressure evolution from the evolved particle distribution function via an appropriate choice of normalisation [7]. Such a decoupling has the potential to make a transition between fluid and kinetic treatments more straightforward, as well as enabling a more efficient treatment of velocity space coordinates. We found that the moment kinetic approach performed comparably to the drift kinetic approach when simulating parallel dynamics with periodic boundary conditions (corresponding to closed field lines) but became problematic when employing wall boundary conditions (corresponding to open field lines) [7]. The genesis of this issue is the combination of two things: the need to impose a wall boundary condition on the particle distribution function that differs for particles with positive and negative parallel velocities, respectively; and the fact that a shifted parallel velocity variable is used in the moment kinetic approach, rendering the true parallel velocity a function of time. One must thus impose a boundary condition at a point in phase space for which in general there will be no corresponding grid point in the code. It is possible that a clever choice of numerical algorithm may overcome this difficulty, but we were unable to devise such an algorithm in the time provided that could solve the problem. One way to avoid this issue would be to separately evolve density and pressure, but not the flow [7]. However, this appears to sacrifice one of the main advantages of the moment kinetic approach: the ability to evolve a potentially closed set of low-order fluid moments. Consequently, we chose to focus on the standard drift kinetic approach when expanding our model to consider helical magnetic fields.

4. Wall boundary condition for the helical magnetic field

As described in [8], inclusion of a radial electric field in the model modifies the wall boundary condition for the ions. In particular, it makes the critical velocity beyond which no ions can be present a function of the time-dependent radial electric field. This introduces a problem similar to the one described above for the wall boundary condition when using the moment kinetic approach. One potential solution – yet to be tried – would be to define a shifted parallel velocity coordinate that absorbs the time dependence of the radial electric field, thus ensuring that the zero of the (shifted) velocity is on the grid and allowing for proper enforcement of the wall boundary condition. In the absence of such a fix, It has been verified that our model works well in the absence of the radial electric field but has poor convergence when the field is included. Solution of this problem is a critical next step necessary to make further progress.

5. Interaction between ions and neutrals

Another of our main goals was to assess the difficulty of treating numerically the interaction between ions and neutrals in the plasma edge. For this purpose we employed relatively simple models for charge exchange and ionisation [7, 8]. The main numerical issue encountered during our investigation was due to the difference in the velocity space dynamics of ions and neutrals: gyrophase information can be averaged away for ions but not for neutral particles. Because the neutrals are not accelerated by the Lorentz force, velocity coordinates aligned with the spatial domain were used. Conversely, the velocity grid for the ions was chosen to align with the magnetic field to take advantage of the lack of gyro-angle dependence. This resulted in the need to perform three-dimensional interpolation in the velocity space when accounting for ion-neutral collisions. One promising way forward would be to use field-aligned velocity coordinates for the neutrals as well. This would eliminate the need for interpolation, provided the ion and neutral velocity coordinates were normalised in the same way. Such a normalisation in itself could lead to numerical inefficiencies if the temperatures of the ions and neutrals are significantly different, as the velocity grid would need narrow spacing to resolve the cold species dynamics and would need to extend to large values to resolve the hot species dynamics. Use of the moment kinetic approach – in which the velocity is normalised by the local species thermal speed – would overcome this but re-introduce the problem of interpolation. A dedicated study of the efficiency of these possible approaches would be beneficial.

6. Extensions to the model

In addition to the outstanding issues raised above, there are numerous extensions that can be made profitably to the current models. The magnetic geometry could clearly be made more realistic by considering full toroidal geometry with a separatrix. The model for electron dynamics (currently an assumed Boltzmann response) could be upgraded. Collisions between different charged particles are currently absent. A more sophisticated treatment of the wall boundary conditions could be employed. Electromagnetic effects are missing. More realistic models for ion-neutral collisions could be used. Toroidal variations in the distribution function could be taken into account.

While there is clearly much that could be done to improve the physics fidelity of the model, we suggest that significant improvements could be made with a few (relatively straightforward) upgrades. Much of the interesting physics of the edge could be explored within a helical magnetic field, provided it is extended to allow for inhomogeneity and for 'flare' in the field lines. Combination with a separatrix-like region to demonstrate transition from open to closed field lines would then provide a fairly complete picture of edge magnetic field geometry. To include such a region would require a more sophisticated treatment for electrons, with possibilities being either a drift-kinetic or fluid treatment. The former could be facilitated by use of a mass ratio expansion so that calculation of the electrostatic potential does not become prohibitively expensive in simulation. A simplified model for charged particle collisions could be used in the first instance to ensure that the equilibrium distribution function is nudged towards a Maxwellian – with the added benefit of aiding possible transition to a fluid treatment.

[1] M. Barnes, F. I. Parra, and M. R. Hardman. Numerical study of 1d drift kinetic models with periodic boundary conditions. *Excalibur/Neptune Report*, 2:2047357–TN–02 M2.1, 2021.

[2] M. Barnes, F. I. Parra, M. R. Hardman, and J. Omotani. Numerical study of 1+1d, moment-based drift kinetic models with periodic boundary conditions. *Excalibur/Neptune Report*, 4:2047357–TN–04 M2.2, 2021.

[3] M. Barnes, F. I. Parra, M. R. Hardman, and J. Omotani. Numerical study of 1+1d, moment-based drift kinetic models with periodic boundary conditions. *Excalibur/Neptune Report*, 6:2047357–TN–06 M2.3, 2021.

[4] M. Barnes, F. I. Parra, M. R. Hardman, and J. Omotani. Numerical study of 1+1d drift kinetic model with wall boundary conditions. *Excalibur/Neptune Report*, 8:2047357–TN–08 M2.4, 2021.

[5] M. Barnes, F. I. Parra, M. R. Hardman, and J. Omotani. Numerical study of 1+1d moment kinetic model with wall boundary conditions. *Excalibur/Neptune Report*, 10:2047357–TN–10 M2.5, 2021.

[6] M. Barnes. Tests for a 2d drift kinetic model for the plasma edge. *Excalibur/Neptune Report*, 12:2047357–TN–12 M1.5, 2021.

[7] M. Barnes, F. I. Parra, M. R. Hardman, and J. Omotani. Numerical study of 1+1d drift kinetic models for parallel dynamics in the plasma edge. *Excalibur/Neptune Report*, 14:2047357–TN–14 D2.2, 2022.

[8] M. R. Hardman, J. Omotani, M. Barnes, and F. I. Parra. Numerical study of a reduced model coupling 2d+2v drift-kinetic ions and 2d-3v kinetic neutrals in a helical magnetic field with wall boundaries. *Excalibur/Neptune Report*, 15:2047357–TN–15 D2.4, 2022.