Fast particle physics in XGC

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Introduction

- The X-point included Gyrokinetic Code (XGC) is a state-of-the-art code for modelling turbulence across the whole plasma volume in Tokamaks and Stellarators [1].
- Our goal is to add fast particle physics into XGC.
- Fast particles are high-energy ions generated by neutral beam injection, nuclear fusion and ion cyclotron resonance heating.
- Their distribution function, f, follows a slowing-down distribution, not Maxwellian (see Fig. 1), creating unique challenges:
  1. XGC uses a scheme where $f = f_M + \delta f$ and f_M is approximately Maxwellian. We need to develop a new scheme where either $f = f_{SD} + \delta f$, where f_{SD} is a slowing-down distribution or use a so-called "Full-F" scheme where $f = f$.
  2. The new scheme must operate simultaneously with the existing scheme, necessitating the restructuring of fundamental code elements.
  3. The current derivation of the quasi-neutral Poisson equation (see Eq. 5) assumes the species are approximately Maxwellian. Incorporating fast particle physics require modifying this equation to account for their non-Maxwellian slowing-down distribution.

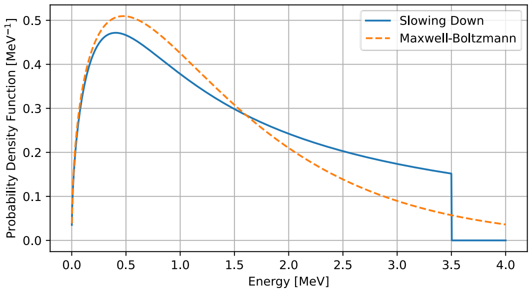

Fig 1. *The solid blue curve shows the slowing-down distribution for thermonuclear alpha particles (derived in e.g. [2]), while the dashed orange curve represents a Maxwell-Boltzmann distribution, with the temperature selected to ensure both distributions share the same mean energy.*

Methods

- We address the first challenge outlined in the introduction, namely, adding "Full-F" capabilities to XGC.
- To validate the new "Full-F" scheme, we conducted tests to ensure it reproduces results from XGC's original scheme.
- While XGC can solve the full electromagnetic gyrokinetic equations with collisions and source terms, for now, we simplify the problem for this work by using the electrostatic gyrokinetic Vlasov equations with adiabatic electrons.
- We tested the new scheme using a Cyclone Base Case scenario as described in [3], a standard benchmark in gyrokinetic simulations.
- The Cyclone Base Case is widely used to validate turbulence models in toroidal magnetic geometries. It features ion-temperature-gradient-driven turbulence in a simplified tokamak with concentric circular flux surfaces.
- The equations we solve are as follows:

Distribtuion function: $f = f(\boldsymbol{R}, u_\parallel, \mu_s)$ (1)

$$\text{Vlasov Equation: } \frac{\partial f}{\partial t} + \frac{\partial f}{\partial \boldsymbol{R}} \cdot \dot{\boldsymbol{R}} + \frac{\partial f}{\partial v_\parallel} v_\parallel = 0 \quad (2)$$

$$\text{Guiding centre eqn: } \dot{\boldsymbol{R}} = \frac{v_\parallel \widehat{\boldsymbol{b}} + \frac{v_\parallel^2}{B} \nabla B \times \widehat{\boldsymbol{b}} + \frac{\boldsymbol{B} \times (\mu \nabla B + \nabla \Phi)}{B^2}}{1 + \frac{v_\parallel}{B} \widehat{\boldsymbol{b}} \cdot \nabla \times \widehat{\boldsymbol{b}}} \quad (3)$$

$$\text{Parallel velocity eqn: } \dot{v}_\parallel = -\frac{(\boldsymbol{B} + v_\parallel \nabla B \times \widehat{\boldsymbol{b}}) \cdot (\mu \nabla B + \nabla \Phi)}{1 + \frac{v_\parallel}{B} \widehat{\boldsymbol{b}} \cdot \nabla \times \widehat{\boldsymbol{b}}} \quad (4)$$

$$\text{Quasi-neutrality: } -\nabla_\perp \cdot \frac{\rho_i^2}{\lambda_{Di}^2} \nabla_\perp \Phi = e(1 - \nabla_\perp \rho_i^2 \nabla_\perp)(\bar{n}_i - n_e) \quad (5)$$

Results: Old vs. New scheme

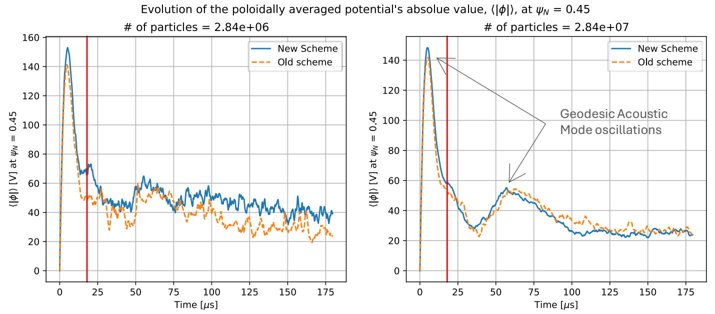

Fig 2. Comparison of the new scheme (solid blue) and the original scheme (dashed orange), showing the mean value of $|\phi|$ along the $\psi_N = 0.45$ flux surface, corresponding to the red circle in Fig. 3. The right panel uses 10 times more particles than the left, resulting in reduced noise.

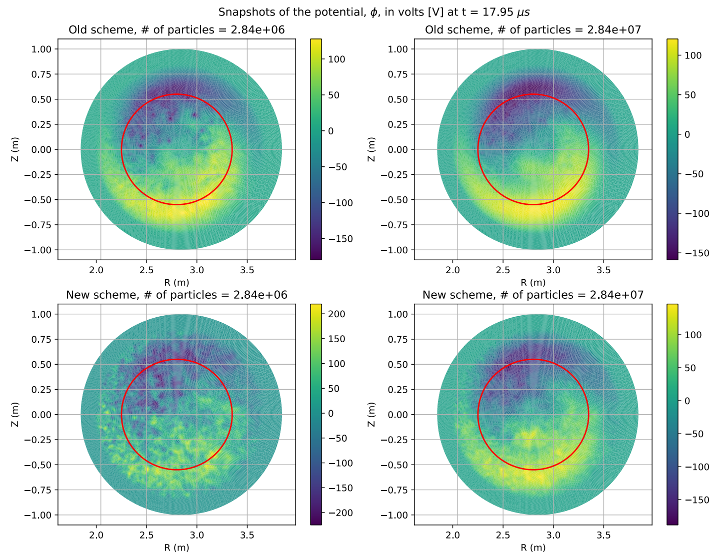

Fig 3. This figure presents snapshots from each of the four simulations used in Fig. 2 at $t = 1.8 \times 10^{-5}$ s, corresponding to the time marked by the vertical red lines in Fig. 2. Each panel shows a cross-section at a specific toroidal angle, with the colour scale representing ϕ in volts.

Numerical Scheme	# of particles	Simulation time
New scheme	2.84×10^6	8.0 hrs
New scheme	2.84×10^7	16.8 hrs
Old scheme	2.84×10^6	14.1 hrs
Old scheme	2.84×10^7	29.6 hrs

Table 1. *Simulation runtimes for each case, performed on the Perlmutter cluster using 4 nodes, each equipped with 4 Nvidia A100 GPUs.*

Discussion and Conclusions

- The results in Fig. 2 are promising, as the new scheme and the old scheme show convergence, particularly in simulations with a higher number of particles.
- The next step is to enhance the new scheme by incorporating additional physics, starting with collisions.
- Table 1 indicates shorter simulation times for the new scheme. However, this is somewhat misleading, as the increased noise in the new scheme requires more markers to achieve comparable accuracy.
- A comparison of the top-right and bottom-right panels in Fig. 2 highlights that the new scheme is inherently noisier than the old scheme.
- While progress has been made, the remaining challenges outlined in the introduction—such as addressing quasi-neutrality and supporting mixed schemes—must be resolved before the code can fully model fast particle physics.

References

[1] Hager et al., *Phys. Plasmas*, **29**(11), 2022.
[2] Wesson, J. & Campbell, D. J., Tokamaks, Oxford Univ. Press, 2011.
[3] Sturdevant, B. J. et al., *Phys. Plasmas*, **28**(7), 2021.

Acknowledgements