Machine Learning Acceleration of Gyrokinetic Simulations of Edge Plasma

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It is well known that the boundary plasma plays a critical role in the performance of tokamak plasma fusion and that it requires extreme-scale computing for kinetic first-principles-based understandings due to the non-Maxwellian and multi-species nature. The non-Maxwellian distribution function demands total-f simulations with ~10,000 particles per cell, as opposed to the low-cost (100 or less particles per cell) delta-f simulations that assumes that the background particle distribution function is Maxwellian. The real cost raiser for a realistic ITER simulation is the necessity for nonlinear Fokker-Planck collision operator in a non-Maxwellian plasma in the presence of wall sputtered impurity particles. For example, Tungsten particles could have tens of different charge states/species which collide with each other in different ways. In the XGC edge gyrokinetic code that uses state-of-the-art Fokker-Planck operation, the cost of the nonlinear Coulomb collision increases as N^2, where N is the number of different plasma and charge species. Without a game-changing improvement of the nonlinear Fokker-Planck algorithm, the Coulomb collision cost can become prohibitively expensive. An accurate digital twin or surrogate model development using machine learning could resolve this issue.

In this work, in collaboration with applied mathematicians, the nonlinear Fokker-Planck operator has been replaced by an encoder-decoder neural network[1,2]. A salient feature of the present neural network is that it is trained specifically to respect conservation properties of the Fokker-Planck collision operator including mass, momentum, and energy, together with the H-theorem, to the accuracy required by the gyrokinetic XGC simulation. Satisfying physics constraint to such a high accuracy has been a difficult problem in the machine learning community. Results of electrostatic turbulence XGC simulations using the machine learning collision operator will be presented, comparing the velocity distribution functions and multiscale edge physics dynamics resulting from the normal and ML-collision solver simulations.

References

[1]M. A. Miller, R.M. Churchill A. Dener et al, “Encoder–decoder neural network for solving the nonlinear Fokker–Planck–Landau collision operator in XGC,” J. Plasma Phys. 87, 905870211 (2021), vol. 87; doi:10.1017/S0022377821000155 (M.A. Miller was a student supervised by Dr. Churchill.)

[2] A. Dener, M.A. Miller, R.M. Churchill et al., “Training neural networks under physical constraints using a stochastic augmented Lagrangian approach,” submitted to Journal of Computational Physics (A. Dener is an applied mathematics postdoc at Argonne National Laboratory working with Dr. Churchill.)