Physics-Constrained Neural Network to replace Expensive Fokker-Planck Solver

A Collaborative Success between SciDAC FASTMath and HBPS

Scientific Achievement

Developed an augmented Lagrangian method for training an encoder-decoder neural network for approximating the collision operator for XGC and other fusion gyrokinetic codes, while conserving mass, momentum & energy

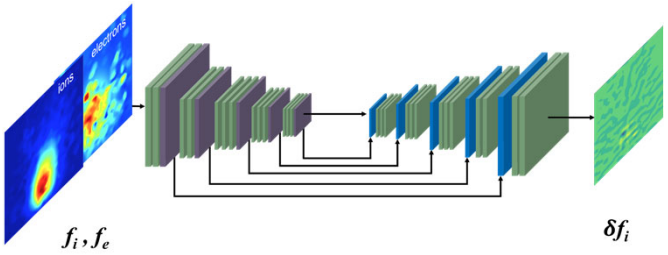
Significance and Impact

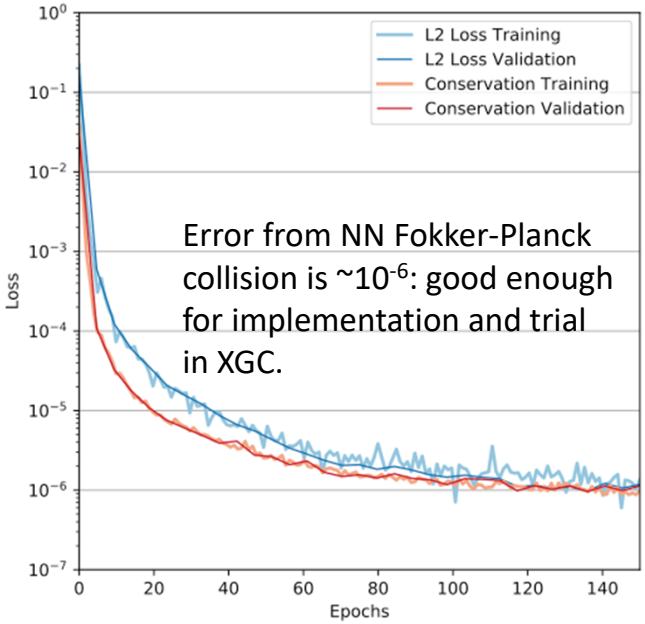
- XGC is a massively parallel particle-in-cell code studying edge turbulence in magnetic fusion energy devices
- ITER plasma will be affected by many tungsten species: Solution time for collision operator does not scale well with number of species and could dominate the exascale computing time
- Showed that a physics-constrained neural network can approximate well the collision operator and conserve required properties, without considering each species separately
- The training time with the augmented Lagrangian method requires only a small number of passes through the data

Research Details

The augmented Lagrangian formulation extends conventional neural network training to incorporate nonlinear constraints with minimal intrusion:

- Subproblems are solved using stochastic gradient descent method
- Applied a heuristic updates for the multipliers and penalty factor using out-of-sample validation information
- Network and training are implemented in PyTorch





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