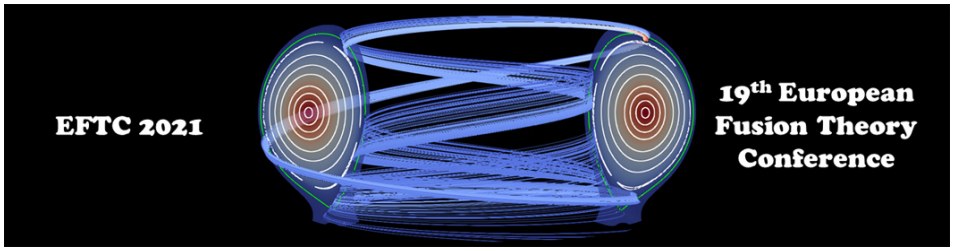

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Machine-learning accelerated Particle-In-Cell Simulations

Tuesday 12 October 2021 14:50 (1h 50m)

Particle-in-cell (PIC) codes are one of the workhorses for numerically exploring plasma dynamics across a vast parameter space. While explicit discretizations of PIC systems allow for a straightforward time integration, stability requirements set strict limitations on both the maximal time-step and maximal grid spacing. Implicit PIC methods on the other hand put laxer restrictions on the time-step and the grid size, but require the solution to demanding linear systems for each time step. In particular, recent work shows that such linear systems are effectively solved using Jacobian-Free Newton-Krylov methods. In this contribution we demonstrate that machine learning can accelerate the GMRES solver, used in time-stepping of the implicit PIC method. To accelerate numerical simulations with machine learning one must determine where predictions from machine learning models can interface with numerical solvers. Also, machine learning models are known to interpolate well and extrapolate poorly. Therefore one must also explore how well a machine learning model can accelerate a simulation, depending on the training data set. To address these fundamental questions, we consider the simplest possible case, 1d electron plasma oscillations. We train neural networks to propose vectors that augment the Krylov space on which GMRES operates. We present an extensive hyperparameter scan over model architectures and explore the performance of multiple loss functions and regularizations for this task. Furthermore, we define a matrix of simulation initial conditions and evaluate model performance for disjoint training and validation sets. As a result, we find that even moderate augmentation GMRES'Krylov space with proposal vectors from machine learning models can reduce the residuals by a factor of 10.

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